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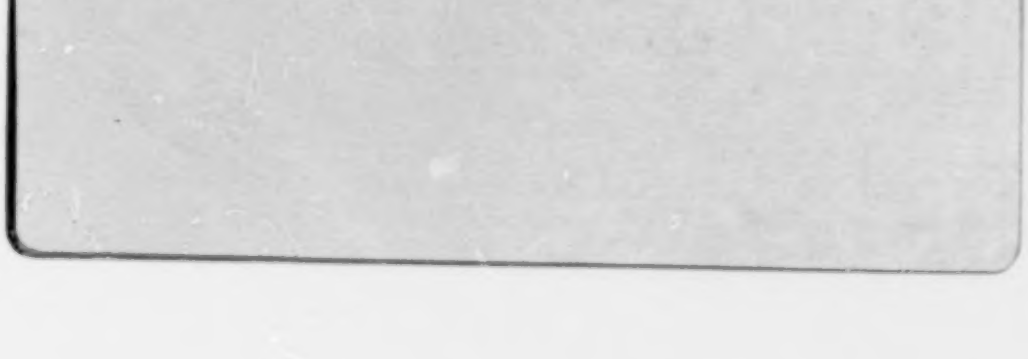

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FINAL TECHNICAL REPORT

ABSORPTION AND EMISSION BY SO_2 BETWEEN 1050 and 1400 cm^{-1} (9.5-7.1 μm)

The work upon which this publication is based was performed pursuant to Contract No. 68-02-0013 with the Environmental Protection Agency
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ABSTRACT

The absorption by the ν_1 (1151.38 cm^{-1}) and ν_3 (1361.76 cm^{-1}) bands of SO_2 has been studied between 1050 and 1400 cm^{-1} (9.5-7.1 μm). Spectral curves of transmittance have been scanned with approximately 1 cm^{-1} resolution for more than 200 samples varying in temperature from about 296 K to 575 K and in pressure from 0.01 to 16 atm. The objective was to provide data on SO_2 absorption and emission that are required to interpret data obtained in this spectral interval on the emission by smokestack exhausts containing SO_2. An extensive table provides information from which the emission between 1050 and 1250 cm^{-1} can be calculated for temperatures between 296 K and 650 K. Water vapor absorbs and emits so strongly in the region of the ν_3 band of SO_2 that this band is probably not useful for remote sensing of smokestacks. Therefore, the ν_1 band was emphasized. The strengths of the two prominent bands in molecules^{-1}cm^{2}cm^{-1} are: ν_1, 371 ± 20 x 10^{-20}; and ν_3, 3020 ± 200 x 10^{-20}.

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SECTION 1

INTRODUCTION AND BACKGROUND

A proposed method of monitoring the SO_2 in the exhaust of smokestacks involves remote sensing of the emission by the SO_2 in the 1050-1400 cm^{-1} (7.1-9.5 μm) region. The absorption bands of SO_2 in this region are sufficiently strong that small concentrations in a typical smokestack produce significant absorptance or emissivity. The Planck function for blackbody radiation is near its maximum in this spectral region for typical exhaust temperatures, and atmospheric paths of a few hundred meters are relatively transparent.

Besides the SO_2 lines, the emission spectrum of the exhaust from a smokestack contains lines due to H_2O and possibly some additional lines due to other combustion products. Carbon-dioxide emission in the region of the SO_2 bands between 8 and 10 μm is probably negligible[1]. The spectrum of the radiation reaching a remote observing station is modified further by the H_2O absorption in the atmosphere. Absorption by other permanent atmospheric gases over paths of a few hundred meters is probably negligible over the spectral region of interest.

The primary objective of the present study has been to provide data on the absorption and emission by SO_2 and H_2O that are required to interpret

emission data from smokestack exhaust containing SO_2. The emphasis has been on quantitative data relating absorption to temperature, path length, concentration of SO_2, and pressure. No work has been done on line identification or line positions. It is anticipated that the spectral features of laboratory data and the integrated emissivity over various portions of the band will be compared with field data on smokestack exhausts. Errors in determining the temperature of the exhaust gas and in accounting for the interference by H_2O in the exhaust and atmosphere will probably result in at least $\pm$ 10 % error in the SO_2 concentrations measured.

Although the primary interest is in emissivity, rather than absorptance or transmittance, we have measured transmittance. Since the gas was in thermal equilibrium, the emissivity ϵ can be found from the transmittance T by $\epsilon = 1-T = A$. The effect of absorption or emission by the windows of the hot cell was accounted for easily by the method used in this study. The radiation beam was chopped between the source and the hot cell so that radiation emitted by the cell was not modulated, and therefore, not detected. Absorption by the windows was accounted for by comparing the spectrum of a sample with a spectrum of the cell evacuated.

The ν_3 band of SO_2, which is centered at 1362 cm^{-1} (7.34 μm) is approximately 8 times stronger than the ν_1 band centered near 1151 cm^{-1} (8.69 μm). Thus, smaller amounts of SO_2 could be detected in the 1362 cm^{-1} band than in the one at lower wavenumbers. However, H_2O absorption and emission are strong enough near the 1362 cm^{-1} band to limit severely its usefulness for smokestack monitoring. For example, we have investigated the emissivity of a laboratory sample of H_2O that corresponds approximately to a smokestack 4 m in diameter with 30 % H_2O at 500 K. The average emissivity of the H_2O in the region of the 1362 cm^{-1} band is approximately 0.8; whereas near the 1151 cm^{-1} band, it is less than 0.2. It is clear that the H_2O emission near the 1362 cm^{-1} band would interfere strongly with measurements of SO_2. Absorption by H_2O in the atmospheric path between the smokestack and the receiver would also interfere more near the 1362 cm^{-1} band than at lower wavenumbers.

Since the 1151 cm^{-1} band shows more promise for smokestack monitoring, we have emphasized it in the present study. Spectral curves of the 1362 cm^{-1} band have been scanned and reduced for room temperature samples covering wide ranges of pressure and path lengths, but no samples have been studied at elevated temperatures. The data obtained for this band have been sufficient to determine the band strength and to produce spectral plots of the absorption coefficient.

It is not practical to obtain data on samples of SO_2, H_2O, and N_2 to simulate all of the smokestack exhausts that might be observed. The concentrations of each of the gases, the dimensions of the plume, and the temperatures may all vary over wide ranges. We have studied SO_2 and H_2O independently with the objective of providing data so that the emission by either of these gases can be calculated over the ranges of temperature, plume dimensions, and concentrations of interest. The simplest adequate method of applying laboratory data appears to be different for the two emitting gases. The results of the SO_2 measurements discussed in Section 3 indicate that at a given temperature and at 1 atm pressure, the observed transmittance is related to the SO_2 concentration by a simple exponential expression within the accuracy required to interpret most field data. The analysis of the data in Section 4 makes use of this simple relationship which is used with the experimental data as a basis for calculations of the emissivity of a variety of samples. The limitations of this method of applying the laboratory data are also discussed in Section 4.

More accurate methods of using the laboratory data to calculate the spectral characteristic of other SO_2 samples could be developed. However, such methods are probably more complex and require a much more detailed knowledge of the parameters of the individual absorption lines than could be obtained during the present project. The method of applying the data that is described in Section 4 is simple and the accuracy is probably consistent with smokestack measurements. Spectral curves have been obtained and reduced for a wide variety of samples not included in this report. These

additional data were compared with those that are shown and will be used in future studies of more sophisticated methods of calculating the transmittance or the emissivity.

A different and more complicated approach is recommended for the application of the H_2O data. Benedict and Calfee[2] have calculated the parameters for all of the significant H_2O lines centered in the spectral region of interest. The tabulated positions of the lines are quite accurate, but the strengths and widths should be checked before these calculated data are applied to field measurements. Section 5 includes some data on H_2O absorption that we have obtained recently in our laboratory as a part of another study under Contract F19628-69-C-0263 with Air Force Cambridge Research Laboratories. The data shown illustrate the influence of water and are typical of those intended for use in checking and adjusting the line strengths and widths tabulated by Calfee and Benedict. Limited data are also given on the H_2O continuum absorption in this spectral region.

The absorber thickness, u, of a gas sample is given by:

$$u \text{ (molecules cm}^{-2}) = 0.269 \times 10^{20} \, (273/\theta) \, p^*(\text{atm}) \, L(\text{atm}) \qquad (1\text{-}1)$$

The temperature, θ, is in Kelvins, and L is the geometrical path length through the sample. The density-equivalent-pressure p* approaches the partial pressure p of the absorbing gas at low pressures. Because of the non-linear relationship between the density of SO_2 and its pressure, p* differs significantly from p at the highest SO_2 pressures used. The vapor pressure of SO_2 limited its maximum pressure to approximately 3 atm; at this pressure and 296 K, p* = 1.03 p for SO_2. At lower pressures and higher temperatures, the difference between p* and p is less. At the H_2O pressures employed, the difference between p* and p for this gas is negligible.

The absorption coefficient due to a single collision-broadened absorption line at a point within a few cm^{-1} of the line center, ν_o, is given by the Lorentz shape:

$$k = \frac{S}{\Pi} \frac{\alpha}{(\nu-\nu_o)^2 + \alpha^2} . \qquad (1\text{-}2)$$

The line strength $S = \int k \, d\nu$ is essentially independent of pressure for the conditions of the present study. The half-width α is proportional to pressure for a given gas mixture at a fixed temperature. We have shown in a previous study[3,4] that the Lorentz equation may require modification for $|\nu-\nu_o|$ greater than a few cm^{-1}. The deviation from the Lorentz shape can probably be ignored in the treatment of the SO_2 data, but it is important in dealing with the H_2O data discussed in Section 5.

At a given wavenumber, there may be appreciable absorption by several lines or by continuum due to pressure induced bands or dimers. The total absorption coefficient κ at a given wavenumber is related by Beer's law to T', the true transmittance that would be observed with infinite resolving power.

$$T' = \exp(-\kappa u), \quad \text{or} \quad (-1/u) \ln T' = \kappa . \qquad (1\text{-}3)$$

Where κ varies rapidly with wavenumber, the finite slitwidth of a spectrometer distorts the spectrum, causing differences between T' and the observed transmittance T. The smoothing of a spectrum by the finite slitwidth causes the observable quantity $(-1/u) \ln T$ to be less than κ near points of maximum κ and more than κ near points of minimum κ. The difference between κ and $(-1/u) \ln T$ at a given wavenumber depends on the amount of structure within the spectral slitwidth and upon the transmittance. When T is different from T', T does not have a simple exponential relationship with u such as that shown in Eq. (1-3). In Section 3, we show typical data that indicate T as observed with 1 cm^{-1} resolution approximately follows the simple exponential dependence on the SO_2 absorber thickness u at pressures of about 1 atm or more. The deviation from the exponential relationship is less than the experimental uncertainty if T is greater than about 20 or 30 %. This simple relationship is ordinarily not valid for gases such as CO_2, N_2O, or H_2O at 1 atm because of the structure in the spectra of these gases. The spectrum of SO_2 contains

many very closely spaced lines with clusters of lines in Q branches with the clusters separated by about 3.5 cm^{-1}. At 1 atm, the lines are broadened enough that there is little structure within regions of a few-tenths of a cm^{-1}. Thus, T observed with 0.1 cm^{-1} is approximately equal to T'.

The integrals $\int T' \, d\nu$ and $\int T \, d\nu$ are equal if the integration is performed over the entire band or over an interval between points where the observed transmittance is independent of slitwidth. However, because of the non-linearity in the relationship between T' and κ, $\int (-\ln T') \, d\nu$ may be greater than $\int (-\ln T) \, d\nu$.

The half-width α of a collision-broadened line is proportional to pressure for a gas mixture in which the fractional concentration of each gas species is held constant. In general, the broadening efficiencies are different for different gases so that each gas species in a mixture must be weighted in proportion to its broadening efficiency when calculating the line half-widths. The concentration of SO_2 in smokestacks is sufficiently low that one can neglect self-broadening; i.e., the collisions of SO_2 molecules with other SO_2 molecules. Collisions of the SO_2 molecules with N_2, H_2O, CO_2 and O_2 will dominate the broadening. In previous studies, we have found that the broadening efficiencies of H_2O, CO_2, and O_2 are within about 30 % of that of N_2 if the absorbing gas is not of the same species as the broadening gas. Therefore, it is probably safe to treat the SO_2 lines in smokestack exhaust as if they were broadened by N_2 at ambient pressure. This assumption is substantiated by data discussed in Section 3 that indicate that the absorption by SO_2 diluted in N_2 at about 1 atm total pressure has only a very weak dependence on line half-width.

Most of the laboratory samples in the present study were pure SO_2 or contained large fractions of SO_2. Therefore, in order to relate the results to dilute mixtures of SO_2 in N_2, we have defined a self-broadening coefficient B and an equivalent pressure P_e which is equivalent to α:

$$P_e = Bp + p_{N_2} = p\,(B-1) + P \, . \qquad (1\text{-}4)$$

The absorber pressure, N_2 pressure, and total pressure are denoted by p, p_{N_2} and P, respectively. Note that $P_e = P = p_{N_2}$ for a very dilute mixture of the absorber in N_2.

We have determined B for SO_2 by a method used previously[5] to measure the self-broadening coefficient for a variety of gases. The method involved two absorption cells of different lengths, one about four times as long as the other. A spectrum of the short cell filled with pure SO_2 was scanned. The longer cell was then filled with SO_2 to a pressure so that the absorber thickness was the same as that in the short cell. Nitrogen was then added to the SO_2 in the longer cell, and spectral curves were scanned for several pressures. By comparing the spectral curves, we determined the total pressure of the $SO_2 + N_2$ mixture whose curve matched that of the short sample. Since the absorption by the two samples was the same and the absorber thicknesses were the same, it follows that the equivalent pressures were equal. The value of B was found from Eq. (1-4) by substituting the values of p and p_{N_2} for the two matching samples. By comparing the spectral curves for a variety of samples, we found that $B = 5 \pm 1$ for SO_2. This is also the value determined previously for H_2O[6]. All values of P_e for either SO_2 or H_2O samples discussed in this report are based on Eq. (1-4) with $B = 5$.

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SECTION 2

EXPERIMENTAL METHODS

Two different grating spectrometers were employed to scan the spectral curves. The majority of the data on the 1151 cm^{-1} band were obtained with a Perkin-Elmer Model E-1 monochromator in the double-pass mode with a spectral resolution of about 1 cm^{-1}. In this system, radiation from a Nernst glower was chopped at 450 Hz and transmitted through a sample cell with NaCl windows to the monochromator. The beam emerging from the monochromator was filtered to eliminate second and higher orders of radiation and was focused onto a helium-cooled, Ge:Cu detector. The detector signal was amplified by a phase-sensitive amplifier and displayed on a strip chart recorder with the chart drive synchronized with the grating drive.

All of the optical path external to the Perkin-Elmer monochromator was enclosed in a plywood box that was flushed with dry nitrogen to reduce absorption by the H_2O in the atmosphere. This method was adequate for the spectral region including the 1151 cm^{-1} band; but absorption by the residual H_2O was still bothersome near the 1362 cm^{-1} band where the H_2O absorption is stronger. Therefore, a different spectrometer with its associated optics enclosed in a vacuum tank was used to study the region containing the 1362 cm^{-1} band. The spectrometer was also double-passed and was coupled to a multiple-pass absorption cell with a base length of

1 meter. The spectrometer and absorption cell were built previously in our laboratory and have been described in detail elsewhere[7]. Samples of H_2O and $H_2O + SO_2$, as well as a few low-pressure samples of pure SO_2 were studied in the multiple-pass cell. Other samples of SO_2 requiring short paths for investigation of the 1362 cm^{-1} band were contained in small cells placed in the optical path between the multiple-pass cell and the spectrometer. During these measurements, the multiple-pass cell was evacuated and adjusted to four passes.

Several absorption cell lengths from 0.102 cm to 416 cm were used in order to investigate the influence of changing either the absorber thickness or the pressure while holding the other of these two parameters constant. All of the absorption cells shorter than 39 cm had windows on both ends and were used single pass. The 39 cm cell was 19.5 cm long and was double passed. An image of the radiation source occurred at the NaCl window on one end of the 39 cm cell. A 20 cm radius-of-curvature concave mirror at the opposite end of the cell formed another image on the window about 1 cm to the side of the input image. The exit image was then focused on the monochromator slits. By double-passing this absorption cell, we were able to use a longer path with uniform cell temperature than was possible with a single-pass cell unless a larger furnace were used. Paths of 416 cm or longer were achieved in the multiple-pass cell with 1 meter base length. An oil manometer measured pressures below about 0.1 atm, an Hg manometer between 0.1 and 2 atm, and a Bourdon-type gauge above 2 atm. The estimated uncertainty in the pressure measurements is about $\pm$ 1 percent.

Apparent adsorption and desorption of SO_2 on the walls of the absorption cells created additional problems in the gas sampling. Typically, after a sample of SO_2 was added to a previously-evacuated absorption cell and the cell was shut off from the gas supply, the pressure in the cell decreased by a few percent within several minutes. This decrease in pressure was observable with the pressure gauges or by the infrared absorption and was attributed to adsorption of the gas on the walls of cell. Part of the

adsorption apparently occurred within a few seconds, but in some instances, a few hours were required for equilibrium to occur. The time required for the pressure to reach equilibrium was decreased by preconditioning the cell. This was accomplished by filling the cell with SO_2 to a pressure about 20 % higher than the final pressure desired. This sample was allowed to remain in the cell for a few minutes while part of it adsorbed on the cell walls. A portion of the sample was then pumped out to the desired pressure.

The fraction of a gas sample adsorbed was dependent upon the temperature, the pressure, the volume-to-surface ratio of the cell, and the history of the cell with regard to the amount of SO_2 in it. When a cell filled with SO_2 was evacuated quickly and closed off, the pressure increased for several minutes, indicating that SO_2 was being desorbed from the cell walls. No adsorption or desorption of N_2 was observable.

Comparisons of the absorption by samples in cells covering a wide range of lengths indicated that there was negligible error due to any SO_2 which might have adsorbed on the inside surfaces of the windows where it could cause additional adsorption. Thus, the errors due to adsorption were limited to those resulting in changes in the SO_2 pressure in the cell. When studying pure SO_2 samples, the adsorption was accounted for by adding gas as required to maintain constant pressure while a spectrum was scanned. This technique was not satisfactory for $SO_2 + N_2$ mixtures because the SO_2 adsorbed faster than the N_2 and changed the mixing ratio of the two gas species.

In order to reduce errors due to adsorption in an $SO_2 + N_2$ mixture, we flowed a pre-mixed sample through the absorption cell at regulated pressure while its spectrum was scanned. Mixtures were made in a 20 liter, stainless steel tank with the inner walls honed to reduce the adsorbing surface. The relatively large volume-to-surface ratio of the tank combined with the smooth walls greatly reduced the fractional adsorption from that observed

with the small cells. The tank was evacuated then preconditioned by the method described above. After the pressure had reached equilibrium at pressure p, N_2 was added to total pressure P, usually 14.6 atm, and the gases were mixed by a fan inside the cell. The mixture in % SO_2 is approximately 100 p:P; as discussed in Section 1, a small correction is required to account for the non-linearity in the relationship between the pressures and the densities of the gases. Although we investigated mixtures as lean as 1 % SO_2, we reduced only the data for samples of 3.9 % SO_2 or richer. The absorption by a sample taken from a freshly-made mixture was indistinguishable from that by a sample of the same pressure taken from the mixture after a large potion had been removed and the remainder had been in the mixing tank for several hours. This result indicates that there was negligible error due to adsorption on the walls of the mixing tank. Spectral curves corresponding to samples of different mixing ratios compared favorably.

Before scanning a spectrum of an $SO_2 + N_2$ mixture, we preconditioned the absorption cell for a few minutes with the pressure in the cell approximately 20 % higher than the sample to be studied. The pressure was reduced to the desired value and a continuous flow from the mixing tank through the absorption cell was established. A modified, natural-gas regulator controlled the pressure while a needle valve on the downstream side of the cell controlled the flow rate. The methods of pressure-regulation and flow control were similar to those used previously in our laboratory[8].

Flow rates varied from about 1 to 30 cm^3/second, depending on the cell size and temperature. At elevated temperatures, the maximum flow rate was limited by the time required for the gas to reach the temperature of the cell. Proper flow rates were determined by monitoring the absorption at various wavenumbers as the rate was varied. Absorption in the wings of the bands increases rapidly with increasing temperature, whereas the opposite is true near the centers of the bands. The absorption at all wavenumbers decreased with decreasing absorber thickness which resulted from adsorption

of the SO_2 in the mixture if the flow rate was too low. Typically, there was a wide range of flow rates high enough to prevent significant errors due to adsorption, yet low enough to permit the gas in the absorption cell to reach thermal equilibrium. No flow was used for samples contained in the multiple-pass cell.

Samples at elevated temperatures with path lengths of 39 cm or less were contained in an absorption cell placed inside a tubular furnace approximately 36 cm long by 8 cm inside diameter. Adjustable end heaters and baffles maintained the temperature constant to less than ± 2 K along the length of the absorption cell. Thermocouples monitored the temperature at different locations on and near the cell. Temperatures were controlled manually by adjusting the voltage across the heating coils. Normally, the cell temperature varied by less than 1 K during the time required to scan a spectrum.

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SECTION 3

EXPERIMENTAL RESULTS FOR SO_2

Two spectral curves obtained for the same SO_2 sample, but with different slitwidths are shown in Fig. 3-1. Shelton et al.[9] have investigated the line structure in this band and have shown that each of the prominent features is a Q branch and consists of a cluster of several individual lines. The curve obtained with the narrower slits contains some structure that is smoothed out by the wider slits, but most of the lines are still unresolved. At a few tenths of an atm of pure SO_2, the lines are collision broadened enough that most of the structure is smoothed out, except for that due to the prominent clusters.

Figure 3-2 shows spectral curves of transmittance and emissivity for three samples having approximately the same absorber thickness, but different pressures. The differences in the curves are due to the collision broadening of the lines. The transmittance curve of the 0.26 atm sample contains much more structure in the strong part of the band than do the curves corresponding to the higher pressures. The average transmittance of the lowest-pressure sample is also significantly higher than the other two, although the absorber thicknesses are nearly the same. The influence of pressure can be explained in terms of the broadening of the many unresolved spectral lines. At P_e = 0.26 atm, the lines are narrow enough that there is still

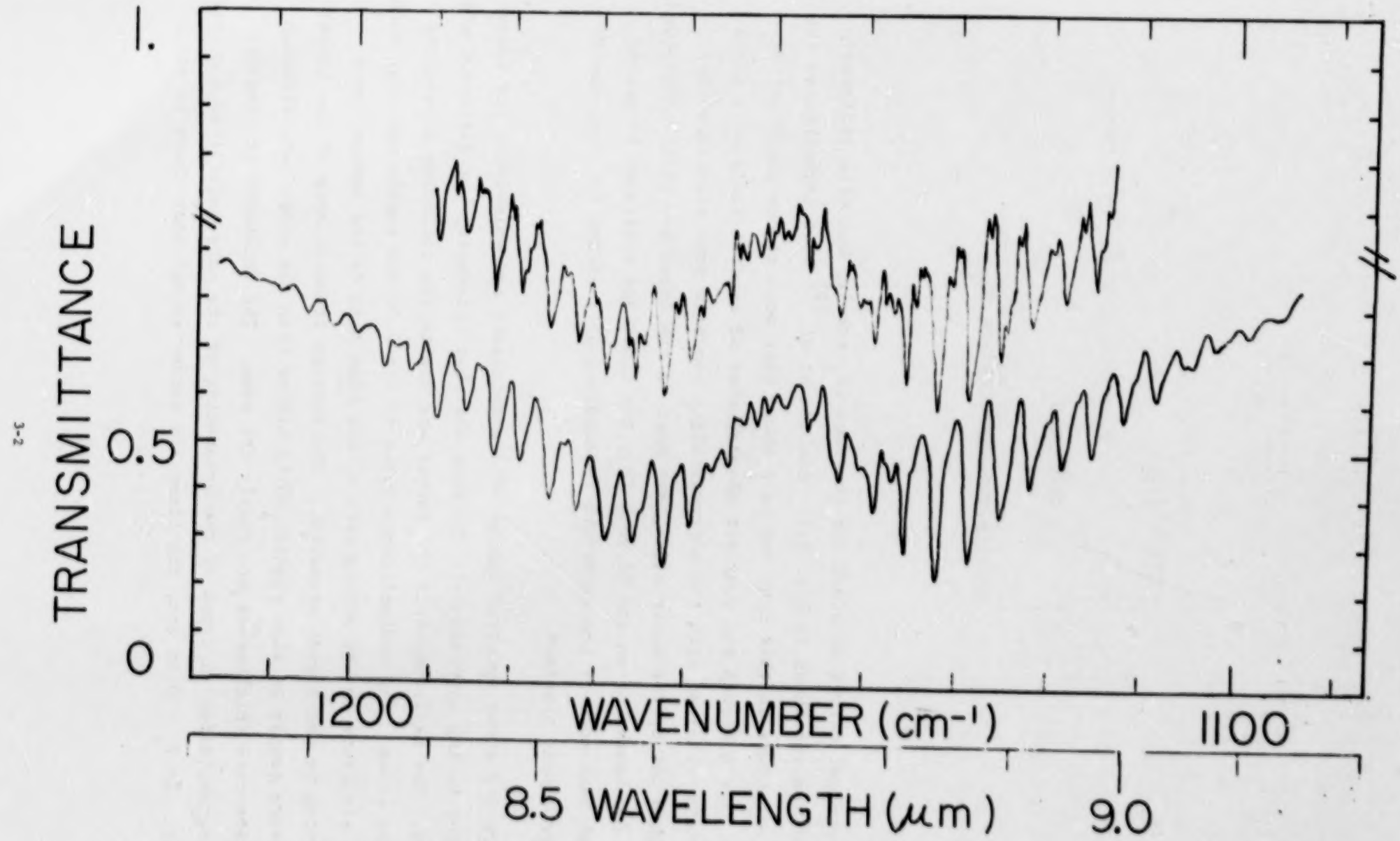


FIG. 3-1. Two spectral curves at different slitwidths for a pure sample of SO_2. The spectral slitwidths for the upper and lower curves are 0.35 and 0.70 cm^{-1}, respectively. The upper curve has been displaced along with its ordinate axis. The sample parameters are: $p = 0.005$ atm; $L = 416$ cm; $u = 0.514 \times 10^{20}$ molecules cm^{-2}, and $\Theta = 297$ K.

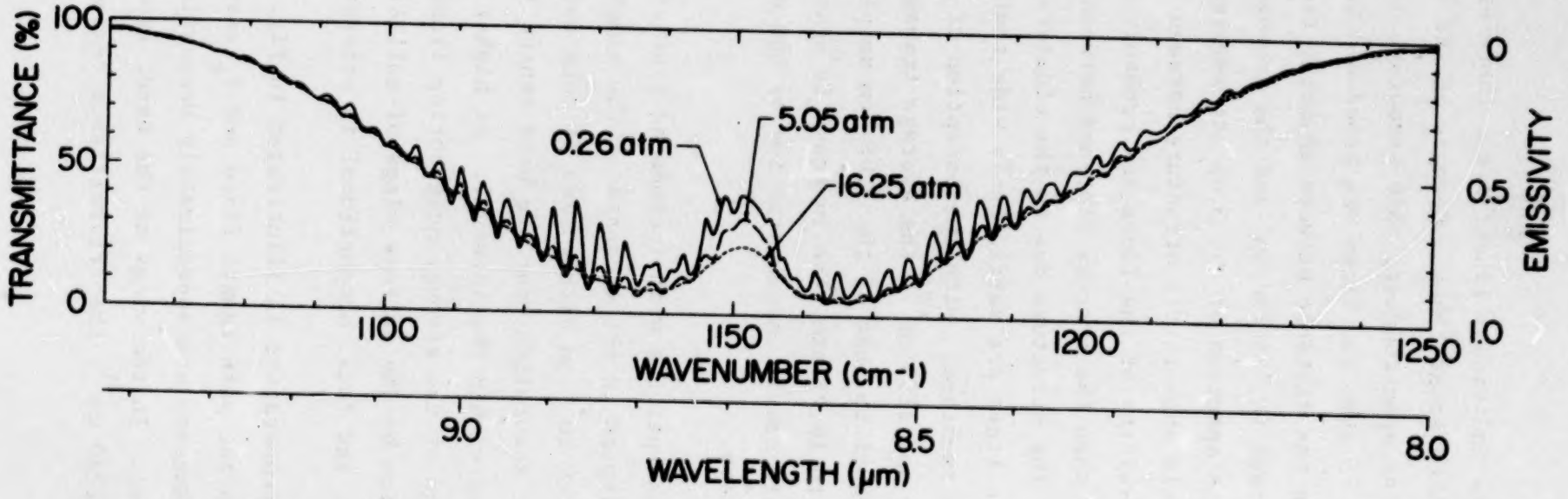


FIG. 3-2. Spectral curves of transmittance between 1060 and 1250 cm^{-1} for three samples of pure SO_2 at different pressures. The values of P_e are indicated. Spectral slitwidth $\tilde{=}$ 1 cm^{-1}, θ = 298 K.

P_e (atm)	L (cm)	u (molecules cm^{-2})
0.26	39.0	4.99 E19
5.05	1.99	4.94 E19
16.25	0.602	4.80 E19

structure due to the individual lines; i.e., there are absorption minima between many of the adjacent lines. Because of the relatively large spectral slitwidth of the spectrometer, this structure does not appear in the curves. At P_e = 5.05 atm, the lines are broadened so that, in most cases, they are wider than the distance between adjacent lines. As a result, the area between the lines is "filled-in" and the average transmittance is less than at 0.26 atm. A spectrum of the 5.05 atm sample scanned with infinite resolving power would show little structure between adjacent lines. At 5.05 atm, the half-widths of the lines are probably between 0.2 and 0.5 cm^{-1}, which is much less than the average distance between the clusters of lines; therefore, some of the structure due to the clusters still remains. At P_e = 16.25 atm, the lines are sufficiently wide that essentially all of the structure has been smoothed. With the exception of the region between approximately 1145 and 1155 cm^{-1}, the average transmittance of the 16.25 atm sample is nearly equal to that of the 5.05 atm sample. As the pressure increases from 5.05 to 16.25 atm, the increase in absorption between the clusters of lines is nearly compensated for by the decrease in absorption near the line centers.

The increase in absorptivity with increasing pressure between 1145 and 1155 cm^{-1} is attributed to the increase in the wings of the very strong lines centered a few cm^{-1} on either side of this interval. At low pressures, most of the absorption near the band center is due to the relatively weak lines centered within the interval. At higher pressures, the contribution by the wings of the strong, neighboring lines becomes appreciable since the absorption by the extreme wings of collision-broadened lines is proportional to α, and thus, proportional to pressure.

The influence of temperature is illustrated in Fig. 3-3, which represents three samples with the path length fixed and P_e essentially constant. Thus, the absorber thicknesses are approximately proportional to the reciprocals of the temperatures. In the wings of the band, from about 1050 to 1090 cm^{-1} and from 1220 to 1250 cm^{-1}, the transmittance decreases with increasing

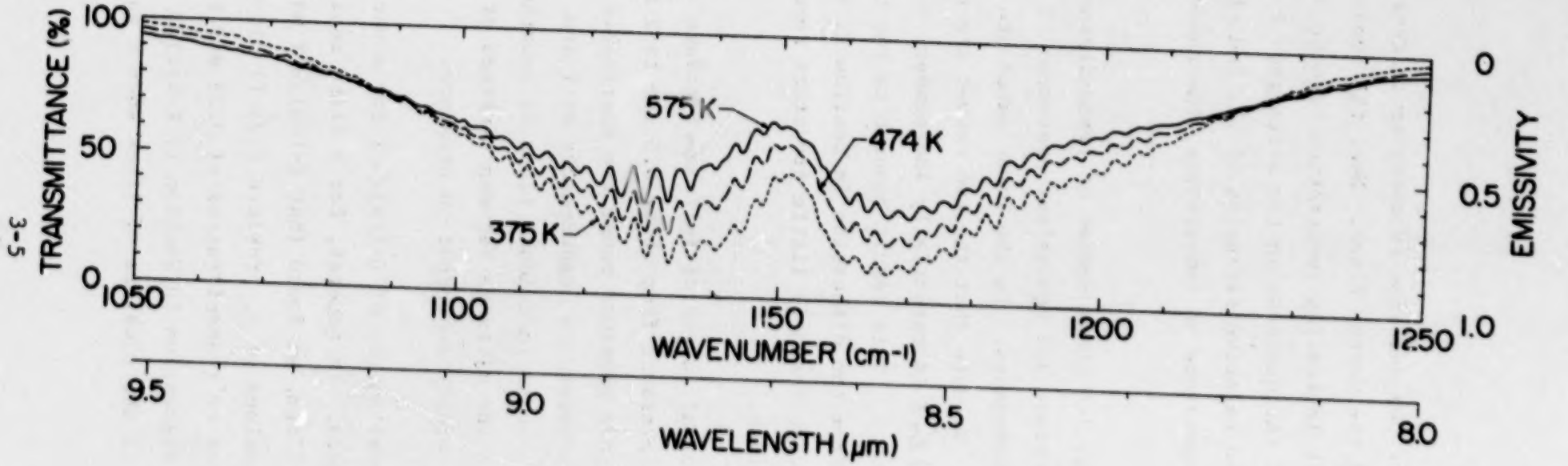


FIG. 3-3. Spectral curves of transmittance between 1050 and 1250 cm^{-1} for three samples of pure SO_2 at different temperatures. $P_e \cong 5.01$ atm. Spectral slitwidth $\cong 1$ cm^{-1}.

Temp. (Kelvins)	L (cm)	u (molecules cm^{-2})
575	1.94	2.49 E19
474	1.99	3.09 E19
375	1.99	3.91 E19

temperature in spite of the decrease in absorber thickness because of the increased strengths of the nearby lines. Near the band center, the transmittance increases with increasing temperature because of the decrease in absorber thickness and the decrease in the strengths of the nearby lines. For a discussion of the relative strengths of the individual lines within a band and of their dependence on temperature, the reader is referred to Refs. (10) and (11).

The upper panel of Fig. 3-4 shows curves of transmittance for two samples having the same temperature and equivalent pressures of about 1.5 atm, but different absorber thicknesses. In the lower panel are the corresponding curves of $(-1/u)\ln T$. We note that the two curves are nearly coincident, indicating that $(-1/u)\ln T$ is essentially independent of u for a rather wide range of values of u. This result amounts to the observed transmittance obeying Beer's law. From the discussion in Section 1, we can conclude that at the pressure involved, there is little structure remaining within an interval of one slitwidth.

The shapes of the spectral curves of $(-1/u)\ln T$ change only slightly with changes in equivalent pressure from about 0.5 atm to 2 atm. Consequently, data obtained within this pressure range are applicable , without accounting for pressure differences, to measurements at 1 atm. At about 1 atm, most of the structure due to individual lines is smoothed, yet the lines are much narrower than the distance between clusters of lines, and the transmittance is only weakly dependent on pressure.

We have compared several curves of $(-1/u)\ln T$ for a variety of pressures and absorber thicknesses. In general, for a fixed equivalent pressure greater than about 0.5 atm, we found that $(-1/u)\ln T$ was essentially constant over a wide range of values of u, provided $(-\ln T)$ did not exceed about 1.5 or 2, corresponding to transmittances of 0.22 and 0.14, respectively. As expected from the discussion in Section 1, $(-1/u)\ln T$ was systematically low near the centers of the clusters of lines when T was less than about

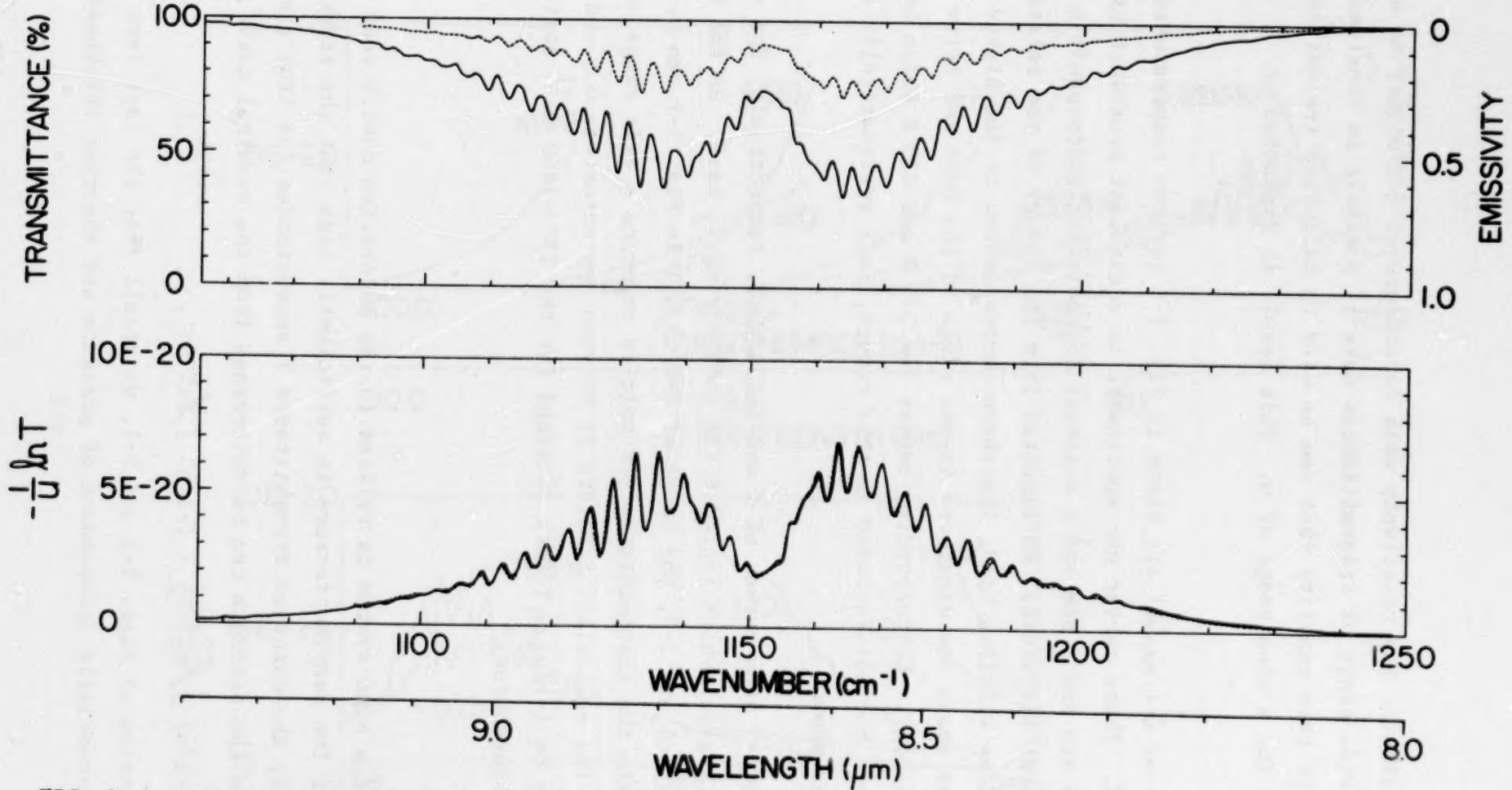


FIG. 3-4. Spectral curves of transmittance and $(-1/u)\ln T$ between 1060 and 1250 cm^{-1} for two samples having different absorber thicknesses. Spectral slitwidth $\simeq$ 1 cm^{-1}. θ = 298 K. The units of $(-1/u)\ln T$ are molecules^{-1} cm^2.

Curve	P_e (atm)	L (cm)	u (molecules cm^{-2})
Broken	1.40	1.99	0.49 E19
Solid	1.59	1.99	1.55 E19

20 % at these points. The relatively weak dependence of $(-1/u)\ln T$ on u observed for a wide range of transmittances make it possible to construct a single curve of this quantity that can be used to calculate transmittances or emissivities for a wide range of u. This result is exploited in Section 4.

Spectral curves of $(-1/u)\ln T$ are shown in Fig. 3-5 for two temperatures, 293 K and 573 K. These curves are applicable to equivalent pressures between about 0.5 atm and 2 atm and a spectral degradiation corresponding to 1 cm^{-1} spectral slitwidth. As expected from the theory of the relative strengths of lines within a band, the curve corresponding to the higher temperature lies above the other one in the wings of the band and below it near the band center. Corresponding curves for 375 K and 475 K which have been constructed, but not included in this report, fall systematically between the curves shown.

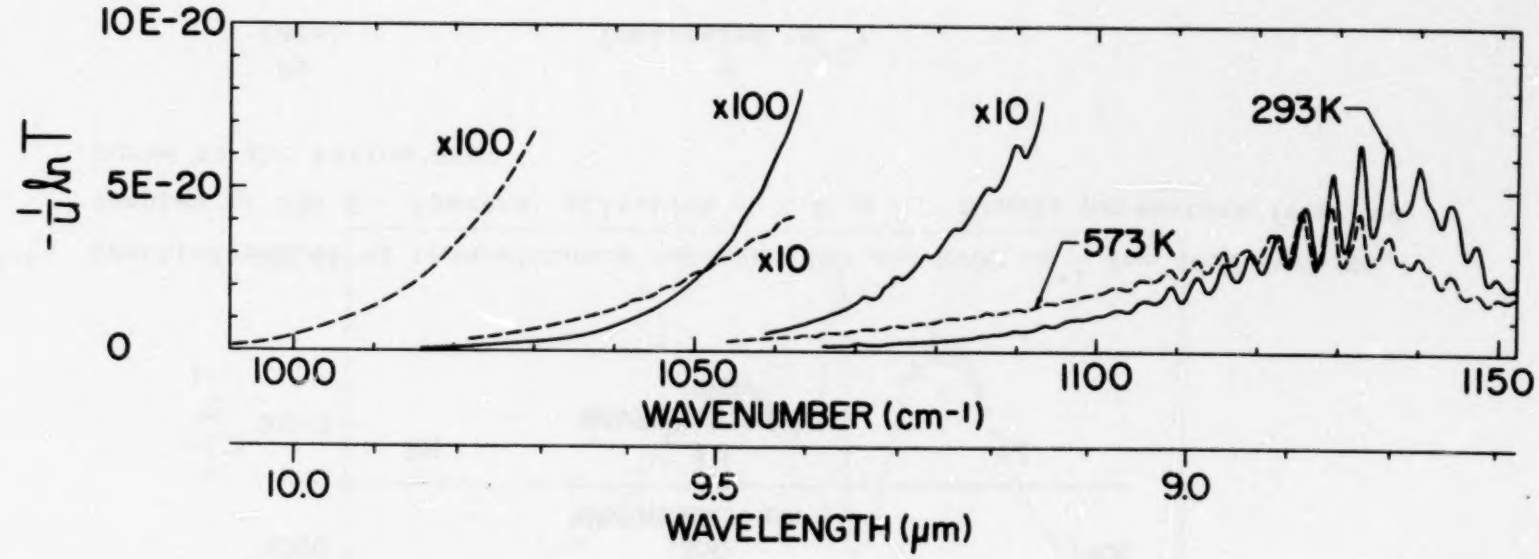
Figures 3-6 and 3-7 show curves of T and $(-1/u)\ln T$, respectively, for the 1300-1400 cm^{-1} region, which includes the very strong ν_3 band. As for the curves in Figs. 3-4 and 3-5, the curve of $(-1/u)\ln T$ in Fig. 3-7 can be used to calculate the transmittance for samples covering a wide range of values of u if the equivalent pressure is between approximately 0.5 and 2 atm. No data on $(-1/u)\ln T$ were obtained for the 1300-1400 cm^{-1} region at elevated temperatures.

BAND STRENGTHS

The strength of a band system is related to the absorption coefficient by $S = \int \kappa \, d\nu$. If the sample pressure is sufficiently high that the structure is smoothed out, the observed transmittance T approximates the true transmittance T' and the strength can be determined from the spectral curve by:

$$S = \int \kappa \, d\nu = (-1/u) \int \ln T' \, d\nu = (-1/u) \int \ln T \, d\nu \, . \qquad (3\text{-}1)$$

From the discussion of Figs. 3-2 and 3-4, we recall that the last term of Eq. (3-1) is essentially independent of pressure and absorber thickness



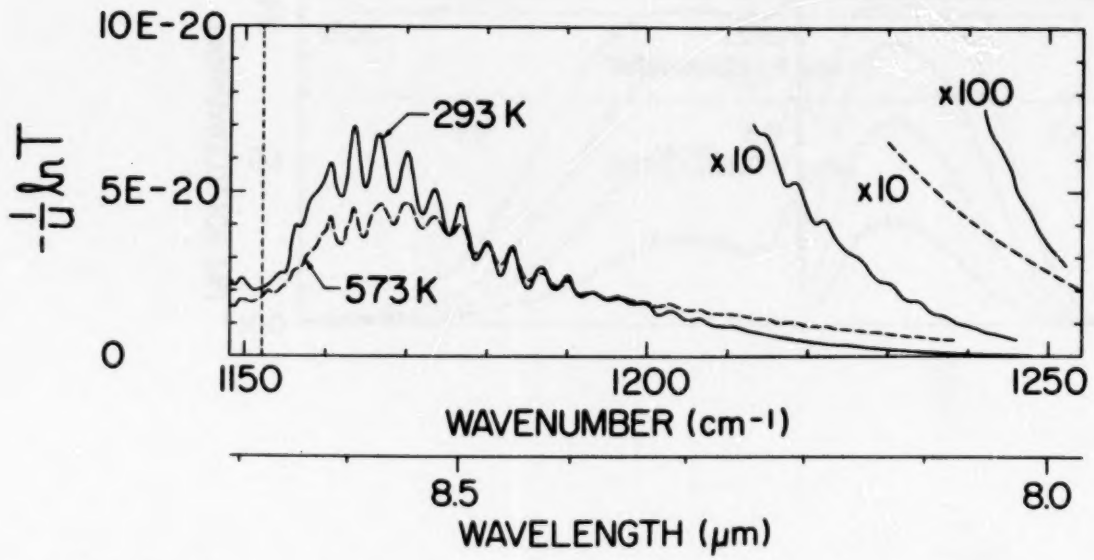


FIG. 3-5. Spectral curves of $(-1/u)\mathcal{L}nT$ between 1000 and 1250 cm^{-1} for two different temperatures. In the wings of the band where the absorption is weak, the values have been multiplied by either 10 or 100, as indicated, before being plotted. Spectral slitwidth $\cong$ 1 cm^{-1}.

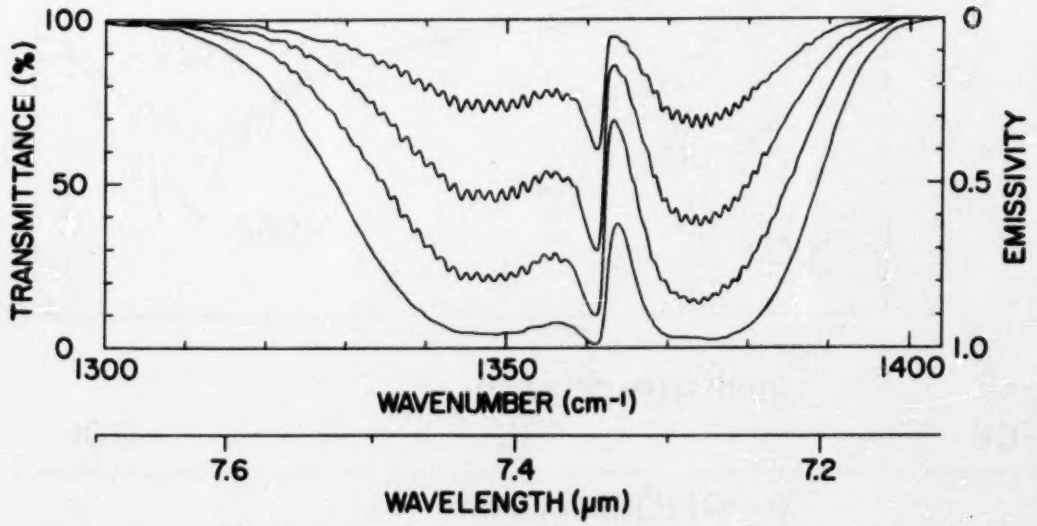


FIG. 3-6. Spectral curves of transmittance between 1300 and 1400 cm^{-1} for four pure SO_2 samples at 296 K. Spectral slitwidth $\simeq$ 1.2 cm^{-1}. Sample parameters from top curve to the bottom are:

Pe (atm)	u (molecules cm^{-2})
1.00	5.03 E17
2.51	12.6 E17
5.04	25.3 E17
10.2	51.1 E17

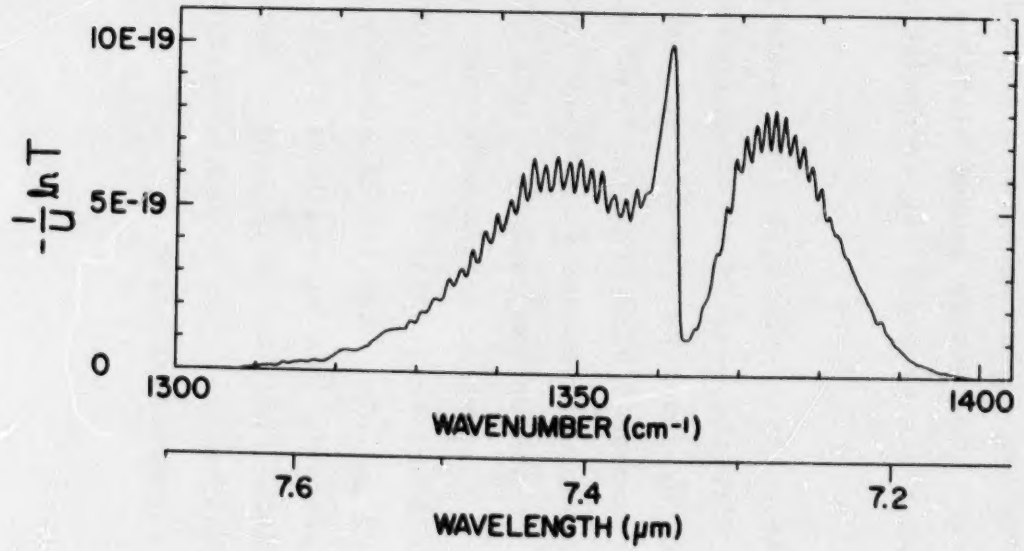


FIG. 3-7. Spectral curve of $(-1/u)\,\ell_\eta T$ between 1300 and 1400 cm^{-1} for temperatures near 296 K and equivalent pressures between 0.5 and 2 atm. Spectral slitwidth = 1.2 cm^{-1}. The units of $(-1/u)\,\ell_\eta T$ are molecules cm^{-2}.

for P_e greater than about 1 atm. Under this condition, Eq. (3-1) is valid and the strengths of the band systems can be determined from spectral curves.

The computer program used in reducing the data calculates the quantity $\int_{\nu'}^{\nu} (-1/u) \ln T \, d\nu$ at several points throughout the spectrum. The lower limit of integration, ν', is at the low wavenumber side of the band. We have compared the computed values of the integral over each of the bands from data on several samples. The results agreed within a few percent for samples with P_e greater than 1 atm provided the transmittance was not less than 20 %.

Table 3-1 summarizes the strengths of the ν_1 and ν_3 bands determined from our data and compares them with the results of other workers. The values listed include contributions by other weak bands that overlap the main band. Our results compare favorably with previous work on both bands. The ν_3 band is difficult to measure because it is very strong and it is necessary to use a very short absorption cell or dilute mixtures of the SO_2 in a non-absorbing gas. Adsorption causes uncertainties in the sampling of dilute mixtures as pointed out in Section 2. Our results are based on samples contained in a 0.102 cm cell. Results obtained with different mixtures agreed within a few percent. The strength of the ν_1 band is essentially independent of temperature, although strengths of many of the individual lines depend strongly on temperature. Any possible variation in the band strength is less than the experimental error.

TABLE 3-1

BAND STRENGTHS

Band	Temp. (K)	Strengths (Multiply all values by 10^{-20} molecules^{-1}cm^{2}cm^{-1}) Present Work	Other Workers	
ν_1				
1151 cm^{-1}	296 K (Room)	371 ± 20	345 ± 35	Eggers and Schmid (Ref.12)
			394 ± 10	Mayhood (Ref.13)
			435 ± 25	Morcillo and Herranz (Ref.14)
	735	373 ± 25		
	475	371 ± 25		
	570	373 ± 25		
ν_3				
1362	296	3020 ± 200	3120 ± 300	Eggers and Schmid (Ref.12)
			3170 ± 90	Mayhood (Ref.13)
			3270 ± 100	Morcillo and Herranz (Ref.14)

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SECTION 4

CALCULATED VALUES OF $(-1/u)\ln T$

We have shown in previous sections that $(-1/u)\ln T$ at a given wavenumber is nearly constant over a wide range of u when $P_e = 1$ and the temperature θ is constant. The experimental data on $(-1/u)\ln T$ are limited to four temperatures: approximately 296 K, 375 K, 470 K, and 573 K. This section deals with calculating $(-1/u)\ln T$ for several other temperatures with the experimental data serving as a basis. The results are presented for 296 K and for thirteen higher temperatures in Table 4-1.

A few different samples were used to provide data for each temperature. The sample used in a particular spectral region was usually chosen so that $(-\ln T)$ was between approximately 0.2 and 1 and could be measured accurately. In the wings of the band where the absorption is very weak, none of the samples produced $(-\ln T)$ as large as 0.2. In these cases, the samples having the largest u were used. The data used were consistent with similar data obtained for other samples, but not included in this report.

Independent calculations were made at points separated by 0.2 cm^{-1} from 1050 to 1250 cm^{-1}. A curve fitting routine was used to fit the experimental data of $(-1/u)\ln T$ to a second order polynomial expressed in terms of $1000/\theta$. Values based on this polynomial were then used to calculate

$(-1/u)\ln T$ (296 K) and the coefficients required to yield the following ratio:

$$R(\theta) = 100\left[\frac{-\ln T}{u}(\theta)\right] \Big/ \left[\frac{-\ln T}{u}(296)\right] = a_o + a_1\left(\frac{1000}{\theta}\right) + a_2\left(\frac{1000}{\theta}\right)^2 \quad (4\text{-}1)$$

Values of $R(\theta)$ were calculated at the thirteen different temperatures listed in Table 4-1. The value of $\frac{-\ln T}{u}$ at θ is denoted by $\frac{-\ln T}{u}(\theta)$.

The ratio in Eq. (4-1) was expressed in terms of the reciprocal of θ, instead of θ, since the reciprocal appears in the expression relating the strengths of individual lines to the band strength. Satisfactory fits could also probably be found if $R(\theta)$ were expressed in terms of θ, instead of $1/\theta$. The factor of 1000 makes the sizes of the coefficients a_o, a_1, and a_2 more convenient than if $1/\theta$ were used. The factor 100 in Eq. (4-1) makes it possible to tabulate values of $R(\theta)$ to an accuracy consistent with the experimental data without using decimal points.

The values of the coefficients a_o, a_1, and a_2 determined from the least-squares fit to the data are included in Table 4-1. Also included is the percentage deviation, to the nearest whole percent, between the experimental data and the calculated values at the same temperatures. From left to right, the four columns under percent error correspond to temperatures of approximately 296 K, 375 K, 475 K, and 573 K.

In some spectral regions where there is structure in the spectrum, $(-1/u)\ln T$ changes by several percent from one data point to the next. Therefore, slight errors in wavenumber calibration may produce sizeable errors in the experimental value at a given wavenumber. These errors are reflected in the calculated values with the result that the uncertainty at a given wavenumber may be much greater than the average uncertainty over an interval of a few cm^{-1}. The greatest errors probably occur on the sides of clusters of lines.

It should be emphasized that the values given in Table 4-1 are based on data obtained with approximately 1 cm^{-1} spectral slitwidth. The true values

of $(-1/u)\ln T$ that would be observed with infinite resolving power would show somewhat more structure; the peaks due to the clusters of lines would be a few percent higher with the valleys between the clusters correspondingly lower. Differences of not more than a few percent probably exist between the true and calculated values of $\int (-1/u)\ln T \, d\nu$ if the integration is performed over an interval of a few cm^{-1} and $(-\ln T)$ does not exceed approximately 1 or 1.5. For larger values of $(-\ln T)$, the calculated values of the integral of the emissivity or absorptance may be larger than those observed. The percent of error is expected to increase with increasing $(-\ln T)$.

The value of $-\ln T$ for a sample of given u' at one of the temperatures included in Table 4-1 can be calculated by:

$$-\ln T\,(\theta) = \frac{u'}{100}\left\{\frac{-\ln T}{u}\,(296)\right\}\left\{100\left[\frac{-\ln T}{u}(\theta)\right] \Big/ \left[\frac{-\ln T}{u}\,(296)\right]\right\}.$$

The quantities in the braces are given in the table. From $(-\ln T)$, other quantities such as transmittance, absorptance, emissivity, etc., can be calculated. If a calculated value is desired at a temperature between two of the temperatures listed, it can be found by interpolation or by substituting the coefficients a_o, a_1, and a_2 into Eq. (4-1). Calculations outside the temperature range (296 K - 650 K) covered by Table 4-1 should be made with caution since no experimental data were obtained at the higher or lower temperatures. The calculated values at 650 K represent a 75 K extrapolation from the highest temperature at which data exist. Further extrapolation might yield sizeable errors. One use of the calculated data in Table 4-1 is illustrated in Figs. 4-1 and 4-2. These figures show spectral plots of the calculated emissivity of various thicknesses of SO_2 at two temperatures, 475 K and 550 K, representative of the exhaust at the top of a smokestack.

TABLE 4-1

CALCULATED $(-1/u)\ln T$ AT VARIOUS TEMPERATURES

ν (cm^{-1})	$\frac{-\ln T}{u}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100 \ln T}{u}(\theta) / \frac{\ln T}{u}(296)$ θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR
1050.0	2.05E-22	169	255	356	467	582	697	811	924	1032	1138	1239	1337	1430	4.8716E+03	-2.9257E+03	4.4794E+02	5 -8 4 -2
1050.2	2.11E-22	163	247	346	455	568	682	794	905	1013	1117	1217	1313	1406	4.8162E+03	-2.9025E+03	4.4592E+02	6 -9 5 -2
1050.4	2.15E-22	161	243	342	449	560	672	783	893	999	1101	1200	1296	1387	4.7559E+03	-2.8679E+03	4.4096E+02	6-10 5 -2
1050.6	2.20E-22	162	243	340	446	555	666	776	883	988	1089	1186	1280	1370	4.6855E+03	-2.8214E+03	4.3337E+02	7-10 5 -2
1050.8	2.21E-22	168	251	348	454	563	673	783	889	993	1093	1190	1283	1371	4.6406E+03	-2.7773E+03	4.2425E+02	6 -9 4 -2
1051.0	2.23E-22	175	259	357	462	571	680	788	894	996	1095	1191	1282	1370	4.5830E+03	-2.7248E+03	4.1375E+02	5 -8 4 -2
1051.2	2.26E-22	179	263	360	464	572	680	786	890	991	1089	1182	1272	1359	4.5074E+03	-2.6667E+03	4.0316E+02	5 -8 4 -2
1051.4	2.31E-22	179	263	360	464	571	679	785	888	989	1086	1179	1269	1355	4.4884E+03	-2.6535E+03	4.0095E+02	6 -9 5 -2
1051.6	2.36E-22	180	263	360	463	570	677	783	886	986	1083	1176	1265	1351	4.4728E+03	-2.6433E+03	3.9930E+02	7-10 5 -2
1051.8	2.40E-22	175	257	352	455	560	666	771	874	973	1069	1161	1250	1335	4.4412E+03	-2.6325E+03	3.9887E+02	8-11 6 -2
1052.0	2.34E-22	172	252	346	448	552	657	761	862	961	1056	1148	1236	1320	4.4066E+03	-2.6174E+03	3.9743E+02	8-11 7 -2
1052.2	2.61E-22	172	252	344	444	547	650	752	852	949	1042	1132	1219	1302	4.3324E+03	-2.5691E+03	3.8964E+02	8-11 7 -2
1052.4	2.67E-22	173	251	343	441	542	644	745	843	938	1030	1119	1204	1286	4.2656E+03	-2.5251E+03	3.8246E+02	8-11 6 -2
1052.6	2.71E-22	173	251	342	439	539	640	739	836	930	1021	1108	1192	1273	4.2089E+03	-2.4870E+03	3.7615E+02	7-11 6 -2
1052.8	2.76E-22	173	250	340	436	534	634	731	827	920	1009	1095	1178	1257	4.1491E+03	-2.4486E+03	3.7003E+02	7-10 6 -2
1053.0	2.81E-22	172	249	337	432	529	627	724	818	910	998	1084	1165	1243	4.0995E+03	-2.4182E+03	3.6537E+02	7-10 6 -2
1053.2	2.86E-22	171	246	333	427	523	620	715	808	899	986	1070	1150	1227	4.0446E+03	-2.3854E+03	3.6048E+02	6-10 5 -2
1053.4	2.93E-22	168	242	327	419	514	609	703	795	884	970	1052	1132	1208	3.9884E+03	-2.3558E+03	3.5663E+02	6 -9 5 -2
1053.6	2.99E-22	167	239	323	413	506	599	691	782	869	953	1035	1113	1187	3.9182E+03	-2.3138E+03	3.5034E+02	5 -9 5 -2
1053.8	3.04E-22	168	239	321	410	500	591	681	769	854	936	1015	1091	1163	3.8142E+03	-2.2437E+03	3.3873E+02	5 -8 4 -2
1054.0	3.07E-22	172	243	324	411	500	590	678	763	847	927	1004	1078	1149	3.7276E+03	-2.1792E+03	3.2721E+02	4 -7 3 -2
1054.2	3.08E-22	176	249	330	416	504	591	677	761	843	921	996	1068	1138	3.6386E+03	-2.1081E+03	3.1400E+02	3 -6 3 -1
1054.4	3.13E-22	178	249	330	415	502	589	674	758	838	916	990	1062	1130	3.6027E+03	-2.0835E+03	3.0984E+02	3 -6 3 -2
1054.6	3.20E-22	178	249	329	414	501	588	674	757	838	915	990	1061	1130	3.6072E+03	-2.0881E+03	3.1078E+02	4 -7 4 -2
1054.8	3.29E-22	177	247	326	411	497	583	668	751	831	908	982	1053	1121	3.5795E+03	-2.0729E+03	3.0871E+02	4 -7 4 -2
1055.0	3.41E-22	174	242	320	404	489	574	657	739	818	894	967	1037	1105	3.5388E+03	-2.0536E+03	3.0656E+02	4 -7 4 -2
1055.2	3.55E-22	169	236	313	394	478	562	645	726	804	879	952	1021	1088	3.5060E+03	-2.0428E+03	3.0625E+02	5 -8 4 -2
1055.4	3.69E-22	164	229	305	385	468	551	633	713	790	865	937	1006	1072	3.4797E+03	-2.0365E+03	3.0668E+02	5 -9 5 -2
1055.6	3.83E-22	162	225	298	377	457	539	618	696	772	845	915	982	1047	3.3985E+03	-1.9901E+03	3.0007E+02	5 -9 5 -2
1055.8	3.97E-22	160	222	293	369	448	527	604	680	754	825	893	958	1021	3.3090E+03	-1.9358E+03	2.9184E+02	5 -9 5 -2
1056.0	4.08E-22	161	221	291	365	441	518	593	666	738	806	872	935	996	3.2017E+03	-1.8642E+03	2.8003E+02	5 -8 5 -2
1056.2	4.20E-22	162	221	289	362	436	510	582	653	722	789	852	914	972	3.0977E+03	-1.7944E+03	2.6850E+02	4 -8 5 -2
1056.4	4.30E-22	161	219	286	357	429	502	573	642	710	775	837	897	954	3.0330E+03	-1.7546E+03	2.6237E+02	4 -8 4 -2
1056.6	4.41E-22	160	217	282	352	423	494	564	632	698	762	823	882	939	2.9825E+03	-1.7253E+03	2.5815E+02	4 -7 4 -2
1056.8	4.38E-22	165	223	289	359	430	500	570	638	703	766	827	885	941	2.9510E+03	-1.6929E+03	2.5129E+02	3 -7 4 -2
1057.0	4.36E-22	170	229	296	365	436	505	575	643	708	770	830	887	942	2.9164E+03	-1.6585E+03	2.4415E+02	4 -7 4 -2
1057.2	4.33E-22	170	230	296	367	439	510	580	648	714	777	838	896	952	2.9581E+03	-1.6862E+03	2.4869E+02	3 -6 3 -2
1057.4	4.29E-22	169	229	296	368	441	513	585	654	721	786	848	907	964	3.0182E+03	-1.7283E+03	2.5591E+02	2 -5 3 -1
1057.6	4.26E-22	174	235	304	376	448	522	593	663	730	794	856	916	972	3.0115E+03	-1.7124E+03	2.5179E+02	2 -5 3 -1
1057.8	4.25E-22	180	243	312	384	457	530	601	670	736	800	861	920	976	2.9768E+03	-1.6755E+03	2.4390E+02	2 -4 2 -1
1058.0	4.37E-22	179	240	308	378	450	520	589	656	721	783	842	899	954	2.8963E+03	-1.6257E+03	2.3620E+02	1 -3 2 -1
1058.2	4.50E-22	177	236	302	371	441	509	577	642	705	766	824	880	933	2.8323E+03	-1.5898E+03	2.3120E+02	1 -3 1 -1
1058.4	4.61E-22	176	235	300	368	436	504	571	635	698	757	815	870	922	2.7942E+03	-1.5670E+03	2.2778E+02	1 -4 2 -1
1058.6	4.72E-22	176	234	298	365	433	500	566	629	690	749	806	860	911	2.7519E+03	-1.5398E+03	2.2343E+02	1 -4 2 -1
1058.8	4.84E-22	178	236	299	365	432	497	562	624	684	741	796	849	899	2.6902E+03	-1.4955E+03	2.1574E+02	1 -4 2 -1
1059.0	4.99E-22	178	235	297	362	427	491	554	615	673	730	783	835	884	2.6309E+03	-1.4577E+03	2.0974E+02	2 -4 2 -1
1059.2	5.21E-22	176	228	289	352	415	478	539	598	655	710	763	813	862	2.5732E+03	-1.4302E+03	2.0664E+02	2 -5 2 -1
1059.4	5.36E-22	175	227	287	349	411	473	533	592	648	702	754	803	851	2.5332E+03	-1.4053E+03	2.0279E+02	2 -5 3 -1
1059.6	5.45E-22	176	231	290	352	414	475	535	592	648	701	752	801	848	2.4982E+03	-1.3757E+03	1.9710E+02	2 -5 3 -2
1059.8	5.57E-22	178	233	292	352	413	473	532	588	643	695	745	793	838	2.4448E+03	-1.3366E+03	1.9019E+02	2 -5 3 -2
1060.0	5.69E-22	178	232	291	350	410	470	527	583	636	687	736	783	827	2.3991E+03	-1.3062E+03	1.8520E+02	2 -5 3 -1
1060.2	5.73E-22	181	235	294	353	413	472	529	583	636	687	735	781	825	2.3713E+03	-1.2822E+03	1.8054E+02	2 -4 2 -1
1060.4	5.75E-22	182	237	295	355	414	473	530	584	637	688	736	782	826	2.3640E+03	-1.2751E+03	1.7906E+02	1 -3 1 -1
1060.6	5.77E-22	182	237	295	355	415	473	530	585	638	689	737	783	827	2.3685E+03	-1.2776E+03	1.7942E+02	1 -3 1 -1
1060.8	5.82E-22	180	234	292	351	411	469	526	581	634	685	733	780	824	2.3752E+03	-1.2878E+03	1.8186E+02	1 -3 1 -1
1061.0	5.86E-22	179	232	290	349	409	467	524	579	631	682	730	776	820	2.3671E+03	-1.2848E+03	1.8165E+02	1 -4 2 -1
1061.2	5.88E-22	179	233	290	349	408	466	523	577	629	679	727	773	817	2.3485E+03	-1.2712E+03	1.7928E+02	2 -4 2 -1
1061.4	5.95E-22	180	234	291	349	407	464	520	573	625	674	721	766	809	2.3102E+03	-1.2444E+03	1.7470E+02	1 -4 2 -1
1061.6	6.00E-22	183	236	293	351	409	465	520	572	623	671	717	761	803	2.2681E+03	-1.2111E+03	1.6851E+02	1 -3 1 -1
1061.8	6.13E-22	182	235	291	348	405	460	514	566	616	663	709	752	793	2.2354E+03	-1.1918E+03	1.6567E+02	1 -3 1 -1
1062.0	6.27E-22	181	232	287	344	399	454	507	558	607	654	698	741	782	2.2001E+03	-1.1725E+03	1.6305E+02	1 -3 2 -1
1062.2	6.51E-22	179	229	282	336	390	443	493	543	590	635	678	718	757	2.1165E+03	-1.1223E+03	1.5552E+02	1 -3 1 -1
1062.4	6.73E-22	179	228	279	331	383	434	483	530	575	618	659	699	736	2.0325E+03	-1.0686E+03	1.4699E+02	1 -3 1 -1
1062.6	6.90E-22	180	228	279	330	380	429	477	523	566	608	648	686	722	1.9681E+03	-1.0244E+03	1.3954E+02	1 -3 1 -1
1062.8	7.08E-22	180	227	277	327	376	424	472	516	557	597	636	672	707	1.9117E+03	-9.8824E+02	1.3379E+02	1 -3 1 -1
1063.0	7.21E-22	181	228	277	327	375	422	468	511	553	593	631	667	701	1.8767E+03	-9.6291E+02	1.2935E+02	1 -3 1 -1
1063.2	7.32E-22	184	232	280	329	377	424	468	511	552	591	628	663	696	1.8351E+03	-9.2918E+02	1.2302E+02	0 -2 0 -1
1063.4	7.56E-22	181	226	274	321	367	412	455	497	536	574	609	643	676	1.7785E+03	-9.0024E+02	1.1940E+02	1 -3 1 -1
1063.6	7.78E-22	178	223	269	315	360	403	445	485	524	561	595	628	661	1.7317E+03	-8.7519E+02	1.1608E+02	1 -4 2 -1
1063.8	7.91E-22	175	219	264	309	354	397	437	479	518	554	589	622	654	1.7353E+03	-8.8536E+02	1.1878E+02	1 -4 2 -1
1064.0	8.08E-22	171	214	259	304	348	392	433	474	512	549	584	617	649	1.7408E+03	-8.9883E+02	1.2170E+02	1 -4 2 -1
1064.2	8.11E-22	170	213	257	302	347	392	432	472	510	547	582	616	647	1.7443E+03	-9.0161E+02	1.2281E+02	1 -4 2 -1
1064.4	8.11E-22	172	215	259	305	349	393	435	475	514	551	586	619	651	1.7488E+03	-9.0141E+02	1.2236E+02	1 -3 2 -1
1064.6	8.13E-22	176	219	264	310	354	397	439	478	516	553	587	620	651	1.7193E+03	-8.7343E+02	1.1666E+02	1 -3 1 -1
1064.8	8.10E-22	179	223	269	314	358	401	442	481	519	555	589	621	652	1.6963E+03	-8.5100E+02	1.1204E+02	1 -3 1 -1
1065.0	8.23E-22	179	224	269	315	359	402	444	483	521	557	591	624	655	1.7055E+03	-8.5639E+02	1.1283E+02	1 -2 1 -1
1065.2	8.34E-22	179	223	268	313	358	401	442	482	519	555	589	622	653	1.7023E+03	-8.5564E+02	1.1288E+02	0 -2 1 -1
1065.4	8.50E-22	179	223	267	312	356	399	439	477	514	549	582	614	644	1.6679E+03	-8.3296E+02	1.0918E+02	0 -2 1 -1
1065.6	8.74E-22	183	227	271	314	357	397	436	473	509	542	574	604	633	1.5917E+03	-7.7483E+02	9.8857E+01	0 -1 0 -1
1065.8	9.13E-22	185	228	271	313	354	393	431	466	500	531	562	590	617	1.5152E+03	-7.2080E+02	8.9366E+01	0 -1 0 -1
1066.0	9.47E-22	189	232	275	316	356	393	429	463	495	525	554	581	606	1.4399E+03	-6.6275E+02	7.8777E+01	0 -1 0 -1
1066.2	9.73E-22	186	229	272	314	353	392	429	462	495	526	555	582	609	1.4684E+03	-6.8482E+02	8.3407E+01	-1 0 -1 0
1066.4	9.95E-22	185	228	271	312	353	391	429	463	496	527	556	584	611	1.4888E+03	-7.0312E+02	8.6459E+01	-2 1 -2 0
1066.6	1.02E-21	182	225	267	308	349	387	424	459	492	523	553	581	608	1.4973E+03	-7.1483E+02	8.9167E+01	-2 2 -2 0
1066.8	1.04E-21	178	219	261	302	342	380	415	451	484	516	546	574	601	1.5001E+03	-7.2616E+02	9.2274E+01	-2 2 -2 0

TABLE 4-I (CONT.)

ν (cm⁻¹)	$\frac{S_{nT}}{u}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100\,S_{nT}}{u}$ (θ) / $\frac{S_{nT}}{u}$ (296) — θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR
1067.0	1.07E-21	175	215	255	295	334	372	408	442	475	506	536	564	590	1.4837E+03	-7.2339E+02	9.2889E+01	-1 1 -2 0
1067.2	1.09E-21	172	211	251	290	329	366	402	436	468	499	529	557	583	1.4770E+03	-7.2555E+02	9.4119E+01	-1 1 -2 0
1067.4	1.11E-21	168	207	246	286	325	362	398	433	465	497	527	555	582	1.4981E+03	-7.4690E+02	9.8590E+01	-1 1 -2 0
1067.6	1.12E-21	167	205	245	285	323	361	398	432	466	497	528	556	584	1.5169E+03	-7.6256E+02	1.0157E+02	-1 1 -2 0
1067.8	1.12E-21	168	207	247	287	326	363	400	435	468	500	530	559	586	1.5170E+03	-7.5979E+02	1.0075E+02	-1 1 -2 0
1068.0	1.11E-21	170	209	249	289	328	366	403	438	471	503	533	562	589	1.5162E+03	-7.5548E+02	9.9539E+01	-1 1 -2 0
1068.2	1.12E-21	193	234	274	311	347	380	411	440	468	494	518	541	562	1.2369E+03	-5.2316E+02	5.5244E+01	1 -3 2 -1
1068.4	1.13E-21	215	258	297	331	362	390	415	439	460	480	498	515	530	9.4350E+02	-2.8370E+02	1.0071E+01	4 -7 6 -3
1068.6	1.14E-21	208	250	289	324	356	385	411	436	458	479	499	517	534	1.0073E+03	-3.4013E+02	2.1183E+01	3 -6 5 -2
1068.8	1.16E-21	200	241	280	315	348	378	406	432	457	479	500	520	538	1.0855E+03	-4.0850E+02	3.4572E+01	2 -4 3 -2
1069.0	1.19E-21	186	226	264	300	335	367	398	426	453	479	503	525	547	1.2228E+03	-5.2831E+02	5.8003E+01	0 -2 1 -1
1069.2	1.22E-21	173	210	248	285	320	355	387	418	448	476	502	528	552	1.3455E+03	-6.3874E+02	7.9944E+01	-1 0 -1 0
1069.4	1.27E-21	168	204	240	276	311	344	376	407	436	464	490	515	538	1.3312E+03	-6.4087E+02	8.1821E+01	-1 0 -1 0
1069.6	1.31E-21	165	200	236	271	306	339	371	401	430	457	483	508	531	1.3202E+03	-6.3904E+02	8.2249E+01	-1 0 -1 0
1069.8	1.33E-21	167	202	238	273	306	339	370	400	428	455	480	504	527	1.2890E+03	-6.1493E+02	7.7843E+01	-1 0 -1 0
1070.0	1.35E-21	168	203	238	272	306	337	368	397	424	450	475	498	521	1.2582E+03	-5.9307E+02	7.4068E+01	0 -1 0 -1
1070.2	1.39E-21	170	204	239	272	304	335	364	392	419	443	467	489	510	1.2051E+03	-5.5501E+02	6.7455E+01	0 -1 0 -1
1070.4	1.42E-21	171	206	240	272	304	333	361	388	413	437	459	481	501	1.1514E+03	-5.1595E+02	6.0603E+01	0 -2 1 -1
1070.6	1.46E-21	167	201	235	267	299	329	357	384	410	434	457	479	500	1.1781E+03	-5.4235E+02	6.6077E+01	0 -1 0 -1
1070.8	1.50E-21	162	195	228	261	292	323	352	379	406	430	454	477	498	1.2100E+03	-5.7462E+02	7.2834E+01	0 -1 0 -1
1071.0	1.54E-21	162	194	227	258	289	319	347	374	400	424	447	469	490	1.1825E+03	-5.5789E+02	7.0295E+01	0 -2 1 -1
1071.2	1.57E-21	162	194	226	258	288	317	344	371	396	419	442	463	483	1.1490E+03	-5.3480E+02	6.6393E+01	1 -3 1 -1
1071.4	1.58E-21	162	194	226	257	287	315	342	368	393	416	438	459	479	1.1325E+03	-5.2414E+02	6.4682E+01	0 -2 1 -1
1071.6	1.58E-21	164	196	228	259	288	317	344	370	394	417	439	460	480	1.1271E+03	-5.1787E+02	6.3299E+01	0 -1 0 -1
1071.8	1.56E-21	165	198	231	262	293	322	350	376	401	425	447	468	488	1.1504E+03	-5.2946E+02	6.4691E+01	-1 0 -1 0
1072.0	1.55E-21	165	198	230	262	293	323	351	378	403	427	450	471	492	1.1683E+03	-5.4077E+02	6.6642E+01	-1 0 -1 0
1072.2	1.57E-21	164	196	229	260	291	320	347	374	399	422	445	466	486	1.1495E+03	-5.3167E+02	6.5416E+01	-1 1 -2 0
1072.4	1.59E-21	164	196	228	259	289	317	345	371	395	418	441	461	481	1.1340E+03	-5.2263E+02	6.4103E+01	-1 1 -2 0
1072.6	1.61E-21	165	197	229	260	289	317	344	369	393	416	437	457	476	1.1016E+03	-4.9776E+02	5.9583E+01	-1 1 -2 0
1072.8	1.63E-21	166	198	229	259	288	315	341	365	388	410	430	450	468	1.0615E+03	-4.6989E+02	5.4843E+01	-1 1 -2 0
1073.0	1.68E-21	165	196	226	256	283	310	335	359	381	402	422	441	459	1.0360E+03	-4.5636E+02	5.3074E+01	-1 1 -2 0
1073.2	1.72E-21	164	194	224	253	280	306	330	354	376	396	416	434	452	1.0153E+03	-4.4551E+02	5.1677E+01	-1 1 -2 0
1073.4	1.76E-21	163	193	222	251	278	303	328	351	373	393	413	431	448	1.0108E+03	-4.4510E+02	5.1949E+01	-1 0 -1 0
1073.6	1.80E-21	161	190	219	247	274	300	324	347	368	389	408	426	443	1.0037E+03	-4.4458E+02	5.2417E+01	-1 0 -1 0
1073.8	1.86E-21	160	189	217	244	271	295	319	341	362	381	400	418	434	9.7328E+02	-4.2661E+02	4.9764E+01	0 -1 0 -1
1074.0	1.91E-21	163	192	220	247	272	296	319	340	361	380	397	414	430	9.3571E+02	-3.9608E+02	4.4016E+01	-1 0 -1 0
1074.2	1.96E-21	163	193	221	248	273	298	320	342	362	381	399	416	432	9.4138E+02	-3.9894E+02	4.4369E+01	-1 1 -2 0
1074.4	2.02E-21	162	191	219	246	272	296	319	340	361	380	398	415	431	9.4215E+02	-4.0153E+02	4.5066E+01	-2 2 -3 0
1074.6	2.12E-21	158	185	212	237	261	285	306	327	347	365	382	399	414	9.1266E+02	-3.9328E+02	4.5208E+01	-1 2 -2 0
1074.8	2.20E-21	154	181	206	231	255	277	299	319	338	356	373	389	404	8.9662E+02	-3.9010E+02	4.5674E+01	-1 1 -1 0
1075.0	2.22E-21	151	177	202	227	251	273	295	315	335	353	370	387	402	9.1396E+02	-4.0855E+02	4.9616E+01	-1 0 -1 0
1075.2	2.23E-21	149	174	200	224	248	271	293	314	334	353	371	388	404	9.3729E+02	-4.2890E+02	5.3595E+01	0 -1 0 -1
1075.4	2.20E-21	148	173	199	224	248	271	294	315	335	354	373	390	406	9.5325E+02	-4.4115E+02	5.5823E+01	0 -1 0 -1
1075.6	2.18E-21	146	171	196	222	246	270	292	314	335	354	373	391	407	9.7303E+02	-4.5845E+02	5.9209E+01	-1 0 -1 0
1075.8	2.19E-21	144	169	194	219	243	267	290	311	332	352	370	388	405	9.7875E+02	-4.6445E+02	6.1078E+01	0 -1 0 -1
1076.0	2.20E-21	144	169	194	218	243	266	289	310	330	350	368	386	403	9.6891E+02	-4.6006E+02	6.0046E+01	0 -1 0 -1
1076.2	2.23E-21	144	169	194	218	242	266	288	310	330	349	368	385	402	9.6314E+02	-4.5588E+02	5.9315E+01	0 -1 0 -1
1076.4	2.27E-21	144	168	193	217	241	264	286	307	327	346	365	382	398	9.5057E+02	-4.4817E+02	5.8134E+01	0 -1 0 -1
1076.6	2.33E-21	144	167	192	215	238	261	282	303	322	341	358	375	391	9.2325E+02	-4.3139E+02	5.5361E+01	0 -1 0 -1
1076.8	2.40E-21	144	167	190	213	236	257	279	298	316	334	351	367	382	8.9260E+02	-4.1219E+02	5.2565E+01	-1 0 -1 0
1077.0	2.48E-21	143	165	188	210	232	253	273	292	310	328	344	360	374	8.6722E+02	-3.9784E+02	5.0545E+01	0 -1 0 -1
1077.2	2.55E-21	143	165	188	210	231	252	271	290	308	324	340	355	370	8.4556E+02	-3.8302E+02	4.8850E+01	0 -1 0 -1
1077.4	2.59E-21	144	166	189	211	232	252	272	290	308	324	340	355	369	8.4010E+02	-3.7802E+02	4.7050E+01	0 -1 0 -1
1077.6	2.63E-21	143	166	188	210	231	252	271	289	307	323	339	354	368	8.3728E+02	-3.7676E+02	4.6924E+01	0 -1 0 -1
1077.8	2.69E-21	143	165	187	209	229	249	268	286	303	319	334	349	362	8.1401E+02	-3.6189E+02	4.4560E+01	-1 0 -1 0
1078.0	2.73E-21	144	166	187	208	229	249	267	284	301	317	332	346	359	7.9961E+02	-3.5185E+02	4.2852E+01	-1 0 -1 0
1078.2	2.76E-21	143	165	187	208	229	249	267	285	302	318	333	347	361	8.0927E+02	-3.5911E+02	4.4153E+01	-1 0 -1 0
1078.4	2.78E-21	143	165	187	208	229	249	267	285	302	318	333	348	361	8.0983E+02	-3.5920E+02	4.4132E+01	-1 1 -2 0
1078.6	2.80E-21	142	164	186	207	228	248	268	286	303	320	335	350	364	8.3353E+02	-3.7786E+02	4.7577E+01	-1 0 -1 0
1078.8	2.81E-21	141	163	185	206	227	247	266	284	302	318	333	348	362	8.2836E+02	-3.7557E+02	4.7353E+01	-1 0 -1 0
1079.0	2.82E-21	141	163	185	206	226	246	264	282	299	315	330	344	358	8.1124E+02	-3.6421E+02	4.5489E+01	0 -1 0 -1
1079.2	2.84E-21	143	164	185	205	224	243	260	277	293	307	321	335	347	7.5671E+02	-3.2538E+02	3.8834E+01	-1 0 -1 0
1079.4	2.87E-21	144	164	184	204	222	239	256	271	286	300	313	325	337	7.1195E+02	-2.9549E+02	3.3850E+01	-1 0 -1 0
1079.6	2.91E-21	142	163	183	202	221	238	255	271	286	300	313	325	337	7.2123E+02	-3.0401E+02	3.5557E+01	-1 0 -1 0
1079.8	2.96E-21	141	162	181	201	219	237	253	269	284	298	311	324	336	7.2280E+02	-3.0742E+02	3.6429E+01	-1 0 -1 0
1080.0	3.01E-21	141	161	180	199	218	235	251	267	281	295	308	321	333	7.1478E+02	-3.0301E+02	3.5868E+01	-1 1 -2 0
1080.2	3.06E-21	142	162	179	198	216	233	250	265	280	294	307	320	332	7.1828E+02	-3.0795E+02	3.6902E+01	-1 1 -2 0
1080.4	3.12E-21	139	158	178	196	215	232	248	264	279	293	306	319	331	7.2300E+02	-3.1345E+02	3.8197E+01	-1 1 -2 0
1080.6	3.18E-21	139	158	178	196	214	231	248	263	278	292	305	317	329	7.1445E+02	-3.0764E+02	3.7227E+01	-1 1 -2 0
1080.8	3.24E-21	139	158	177	196	213	231	248	263	278	292	305	318	330	7.0161E+02	-2.9911E+02	3.5825E+01	-1 2 -3 0
1081.0	3.33E-21	139	158	177	195	212	229	244	258	272	285	297	309	321	6.7439E+02	-2.8954E+02	3.4713E+01	-1 1 -2 0
1081.2	3.41E-21	140	159	177	194	211	228	241	255	268	281	292	303	314	6.4844E+02	-2.8137E+02	3.4491E+01	-1 1 -2 0
1081.4	3.47E-21	141	159	177	194	210	226	239	252	265	277	288	299	309	6.2345E+02	-2.6370E+02	3.4044E+01	-1 1 -2 0
1081.6	3.54E-21	139	157	175	191	207	222	235	248	261	272	283	293	303	6.0773E+02	-2.5767E+02	3.5864E+01	-1 0 -1 0
1081.8	3.62E-21	138	156	173	189	204	219	232	245	257	268	279	289	299	6.0833E+02	-2.5965E+02	3.9195E+01	0 -1 0 -1
1082.0	3.69E-21	137	155	171	187	202	216	230	242	254	265	276	286	295	5.9353E+02	-2.5321E+02	3.5790E+01	0 -1 0 -1
1082.2	3.74E-21	135	152	169	185	200	214	228	241	253	265	276	286	296	6.0982E+02	-2.6791E+02	3.8714E+01	0 -1 0 -1
1082.4	3.78E-21	134	151	167	183	199	214	228	242	254	267	278	289	299	6.3551E+02	-2.8849E+02	4.2553E+01	0 -2 1 -1
1082.6	3.74E-21	133	151	168	185	201	216	231	245	258	271	283	294	305	6.6826E+02	-3.0892E+02	4.5249E+01	0 -2 1 -1
1082.8	3.73E-21	132	150	167	184	200	216	232	246	260	273	285	297	308	6.8278E+02	-3.1939E+02	4.8038E+01	0 -1 0 -1
1083.0	3.70E-21	134	152	169	186	202	218	233	247	260	273	285	296	307	6.6174E+02	-2.8364E+02	3.4739E+01	0 -1 0 -1
1083.2	3.70E-21	136	154	171	188	203	219	232	246	258	270	281	292	302	6.2466E+02	-2.5501E+02	2.9914E+01	0 -2 1 -1
1083.4	3.79E-21	136	152	169	185	200	214	227	240	252	263	274	284	293	5.9813E+02	-2.4009E+02	2.7419E+01	0 -2 1 -1
1083.6	3.87E-21	136	152	168	183	198	211	224	236	248	258	268	278	287	5.7192E+02	-2.2275E+02	2.4587E+01	0 -2 1 -1
1083.8	3.94E-21	135	152	167	182	197	210	223	235	246	256	266	275	284	5.6379E+02	-2.1819E+02	2.3953E+01	0 -2 1 -1

TABLE 4-1 (CONT.)

ν (cm^{-1})	$-\frac{1}{u}\frac{\partial u}{\partial T}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100}{u}\frac{\partial u}{\partial T}(\theta) / \frac{1}{u}\frac{\partial u}{\partial T}(296)$ θ (Temperature in Kelvins)												COEFFICIENT			% ERROR			
		350	375	400	425	450	475	500	525	550	575	600	625	650	a_0	a_1	a_2				
1084.0	4.03E-21	134	150	166	180	194	208	220	232	243	253	263	272	281	5.5964E+02	-2.1822E+02	2.4321E+01	0	-1	0	-1
1084.2	4.14E-21	132	148	163	178	192	205	217	229	240	251	260	270	279	5.6369E+02	-2.2484E+02	2.5925E+01	0	-1	0	-1
1084.4	4.22E-21	132	148	163	178	192	205	218	229	241	251	261	271	280	5.6866E+02	-2.2844E+02	2.6559E+01	-1	0	-1	0
1084.6	4.27E-21	133	149	164	179	193	206	218	230	241	251	261	270	279	5.5860E+02	-2.1976E+02	2.4870E+01	-1	0	-1	0
1084.8	4.34E-21	134	149	164	179	192	205	217	229	239	249	259	268	276	5.4374E+02	-2.0890E+02	2.2956E+01	-1	0	-1	0
1085.0	4.42E-21	134	150	165	179	192	205	216	227	238	248	257	265	274	5.3102E+02	-1.9991E+02	2.1408E+01	-1	0	-1	0
1085.2	4.50E-21	134	150	165	178	192	204	216	226	237	246	255	264	272	5.2218E+02	-1.9383E+02	2.0385E+01	-1	0	-1	0
1085.4	4.58E-21	134	149	164	177	190	203	214	225	235	244	253	261	269	5.1454E+02	-1.8973E+02	1.9841E+01	-1	0	-1	0
1085.6	4.68E-21	133	148	163	176	189	201	212	223	232	242	250	258	266	5.0721E+02	-1.8627E+02	1.9458E+01	-1	0	-1	0
1085.8	4.78E-21	132	147	161	174	187	198	209	220	230	239	247	256	263	5.0506E+02	-1.8767E+02	2.0062E+01	-1	0	-1	0
1086.0	4.87E-21	131	145	159	172	184	196	207	218	228	237	245	254	261	5.0705E+02	-1.9189E+02	2.1137E+01	-1	1	-2	0
1086.2	4.93E-21	130	144	158	171	183	194	205	215	224	233	242	250	257	4.9291E+02	-1.8358E+02	1.9913E+01	-1	1	-2	0
1086.4	4.93E-21	132	146	159	171	183	194	204	214	223	232	239	247	254	4.7255E+02	-1.6806E+02	1.7103E+01	-1	1	-2	0
1086.6	4.91E-21	132	146	159	172	183	194	204	213	221	230	237	244	251	4.5395E+02	-1.5419E+02	1.4628E+01	-1	1	-2	0
1086.8	4.87E-21	133	147	160	172	183	194	203	212	220	228	236	242	249	4.4028E+02	-1.4379E+02	1.2748E+01	-1	0	-1	0
1087.0	4.82E-21	134	148	161	174	185	195	205	214	222	230	237	244	250	4.3651E+02	-1.3887E+02	1.1622E+01	-1	0	-1	0
1087.2	4.85E-21	134	148	161	173	184	194	204	213	221	229	236	243	249	4.3701E+02	-1.4033E+02	1.2011E+01	-1	0	-1	0
1087.4	4.91E-21	132	146	159	171	182	193	203	212	221	229	236	244	250	4.3538E+02	-1.5625E+02	1.5112E+01	0	-1	0	-1
1087.6	4.97E-21	129	143	156	169	181	192	202	212	221	230	238	246	253	4.8588E+02	-1.8131E+02	1.9858E+01	0	-1	0	-1
1087.8	5.07E-21	128	141	154	167	179	190	201	211	221	230	238	246	254	5.0213E+02	-1.9594E+02	2.2766E+01	0	-1	0	-1
1088.0	5.17E-21	127	140	153	165	177	189	199	209	219	228	237	245	252	5.0863E+02	-1.9653E+02	2.3873E+01	0	-2	1	-1
1088.2	5.26E-21	127	140	153	165	177	188	198	208	218	226	235	243	250	4.9208E+02	-1.9108E+02	2.2208E+01	0	-2	1	-1
1088.4	5.36E-21	128	141	153	165	176	187	197	207	216	224	232	240	247	4.7465E+02	-1.7828E+02	1.9945E+01	0	-2	1	-1
1088.6	5.48E-21	128	141	154	165	176	187	196	206	214	222	230	237	244	4.5528E+02	-1.6394E+02	1.7398E+01	0	-2	1	-1
1088.8	5.59E-21	130	142	155	166	177	187	196	205	213	221	228	235	242	4.3840E+02	-1.5054E+02	1.4910E+01	0	-1	1	-1
1089.0	5.74E-21	130	143	155	167	177	187	196	204	212	219	226	232	238	4.1937E+02	-1.3623E+02	1.2343E+01	0	-1	0	-1
1089.2	5.87E-21	131	144	156	167	177	186	195	203	210	217	223	229	235	3.9621E+02	-1.1879E+02	9.2098E+00	-1	0	-1	0
1089.4	6.02E-21	132	144	156	166	176	185	193	200	207	214	220	225	231	3.7850E+02	-1.0709E+02	7.2981E+00	-1	0	-1	0
1089.6	6.19E-21	129	141	152	163	172	181	189	197	204	210	217	222	228	3.8745E+02	-1.1889E+02	1.0006E+01	-1	1	-2	0
1089.8	6.22E-21	128	140	152	162	172	181	189	197	204	211	218	224	229	3.9872E+02	-1.2769E+02	1.1622E+01	-1	1	-2	0
1090.0	6.27E-21	126	138	149	160	170	179	188	197	204	212	219	225	231	4.2317E+02	-1.4852E+02	1.5848E+01	-1	0	-1	0
1090.2	6.23E-21	125	137	149	160	170	180	189	197	206	213	220	227	234	4.3792E+02	-1.5962E+02	1.7640E+01	-1	0	-1	0
1090.4	6.14E-21	124	136	147	158	169	179	188	197	205	213	221	228	235	4.5190E+02	-1.7166E+02	1.9980E+01	0	-1	0	-1
1090.6	6.04E-21	123	135	146	157	168	178	188	197	206	214	222	229	236	4.6589E+02	-1.8314E+02	2.2152E+01	0	-1	0	-1
1090.8	5.95E-21	123	135	147	158	169	179	188	198	206	215	222	230	237	4.6404E+02	-1.8079E+02	2.1618E+01	0	-1	0	-1
1091.0	5.88E-21	124	136	147	158	169	179	189	198	207	215	223	230	237	4.6093E+02	-1.7771E+02	2.0978E+01	0	-1	0	-1
1091.2	5.96E-21	122	134	145	156	167	177	186	195	204	212	220	227	234	4.6344E+02	-1.8295E+02	2.2310E+01	-1	0	-1	0
1091.4	6.06E-21	120	131	143	154	165	175	185	194	204	212	220	228	236	4.8448E+02	-2.0134E+02	2.5911E+01	-1	0	-1	0
1091.6	6.20E-21	119	129	140	152	163	173	184	193	203	212	220	228	236	4.9878E+02	-2.1448E+02	2.8547E+01	-1	0	-1	0
1091.8	6.29E-21	119	130	141	153	164	174	185	195	204	213	221	229	237	4.9851E+02	-2.1280E+02	2.8372E+01	-1	0	-1	0
1092.0	6.37E-21	120	131	142	154	165	175	186	195	205	213	222	230	237	4.9372E+02	-2.0794E+02	2.7854E+01	-1	1	-2	0
1092.2	6.47E-21	120	132	143	154	165	175	185	195	204	213	221	229	236	4.8486E+02	-2.0122E+02	2.5840E+01	-1	0	-1	0
1092.4	6.56E-21	121	132	143	155	165	176	186	195	204	213	221	229	236	4.8174E+02	-1.9821E+02	2.5224E+01	-1	1	-2	0
1092.6	6.65E-21	121	132	143	155	166	176	186	196	205	214	222	230	238	4.8840E+02	-2.0266E+02	2.5958E+01	-1	2	-3	0
1092.8	6.86E-21	119	130	141	152	163	174	184	193	202	211	219	227	234	4.8559E+02	-2.0399E+02	2.6597E+01	-1	2	-3	1
1093.0	7.28E-21	117	127	137	147	157	167	176	185	194	202	210	217	224	4.6329E+02	-1.9520E+02	2.5950E+01	-1	2	-3	1
1093.2	7.64E-21	115	124	133	143	152	161	170	179	187	194	202	209	215	4.4434E+02	-1.8759E+02	2.5357E+01	-1	2	-3	1
1093.4	7.90E-21	114	122	131	140	149	158	166	174	182	189	196	203	209	4.2899E+02	-1.7995E+02	2.4442E+01	-1	2	-3	0
1093.6	8.11E-21	114	122	130	139	148	156	164	171	179	186	192	199	205	4.1160E+02	-1.6930E+02	2.2811E+01	-1	1	-2	0
1093.8	8.14E-21	115	124	132	141	149	157	164	171	178	184	191	196	202	3.8752E+02	-1.4976E+02	1.9138E+01	-1	1	-2	0
1094.0	8.14E-21	117	126	134	143	150	159	165	172	178	184	190	195	200	3.6481E+02	-1.3056E+02	1.5444E+01	-1	0	-2	0
1094.2	7.92E-21	120	130	139	147	155	163	170	177	183	189	194	200	205	3.5971E+02	-1.2036E+02	1.2871E+01	-1	1	-2	0
1094.4	7.70E-21	123	134	143	152	160	169	175	182	188	194	199	204	209	3.5460E+02	-1.1007E+02	1.0273E+01	-1	1	-2	0
1094.6	7.58E-21	125	135	145	154	162	170	178	184	191	197	202	207	212	3.5905E+02	-1.1048E+02	1.0006E+01	-1	1	-3	0
1094.8	7.45E-21	126	137	147	156	165	173	180	187	194	200	205	211	216	3.6375E+02	-1.1094E+02	9.7300E+00	-1	2	-3	1
1095.0	7.70E-21	123	133	143	152	160	169	176	183	189	195	201	206	211	3.6722E+02	-1.1928E+02	1.1895E+01	-2	3	-4	1
1095.2	7.97E-21	121	130	139	148	156	164	171	178	185	191	196	202	207	3.6825E+02	-1.2561E+02	1.3676E+01	-2	4	-5	1
1095.4	8.26E-21	119	128	137	145	153	161	168	174	181	187	192	198	203	3.6449E+02	-1.2688E+02	1.4383E+01	-2	3	-4	1
1095.6	8.55E-21	118	126	135	143	151	159	165	171	177	183	189	194	199	3.5714E+02	-1.2474E+02	1.4393E+01	-2	3	-4	1
1095.8	8.93E-21	115	123	131	138	146	152	159	165	171	177	182	187	192	3.4940E+02	-1.2551E+02	1.5300E+01	-1	3	-4	1
1096.0	9.34E-21	112	119	127	134	140	147	153	159	165	171	176	181	185	3.4324E+02	-1.2771E+02	1.6489E+01	-1	3	-4	1
1096.2	9.64E-21	111	118	124	131	137	144	150	155	161	166	171	176	180	3.3298E+02	-1.2405E+02	1.6307E+01	-1	2	-3	1
1096.4	9.90E-21	111	117	123	129	135	141	147	153	158	163	167	172	176	3.2139E+02	-1.1794E+02	1.5512E+01	-1	2	-3	1
1096.6	9.97E-21	111	118	124	130	136	142	147	152	157	162	167	171	175	3.1131E+02	-1.0971E+02	1.3961E+01	-1	1	-3	0
1096.8	9.89E-21	113	119	126	132	138	144	149	154	159	164	168	172	176	3.0522E+02	-1.0253E+02	1.2369E+01	-1	1	-3	0
1097.0	9.64E-21	114	121	128	134	140	146	151	156	161	165	170	174	178	3.0325E+02	-9.6233E+01	1.0940E+01	-1	1	-2	0
1097.2	9.82E-21	115	122	129	136	142	147	153	158	163	167	171	175	179	2.9766E+02	-9.1984E+01	9.9198E+00	-1	1	-2	0
1097.4	9.78E-21	116	124	131	137	143	149	155	160	164	169	173	177	180	2.9369E+02	-8.6773E+01	8.7018E+00	-1	1	-2	0
1097.6	9.79E-21	118	125	133	139	145	151	156	161	166	170	174	178	181	2.8755E+02	-7.9467E+01	7.1498E+00	-1	0	-1	0
1097.8	9.78E-21	119	127	134	141	147	153	158	163	168	172	176	179	183	2.8325E+02	-7.3969E+01	5.8377E+00	-1	0	-1	0
1098.0	9.74E-21	119	127	135	142	148	154	160	165	170	174	179	183	186	2.8812E+02	-8.1831E+01	7.4954E+00	-1	0	-1	0
1098.2	9.71E-21	119	127	135	142	149	155	161	166	172	176	181	185	189	3.1241E+02	-9.3854E+01	9.1711E+00	-1	0	-2	0
1098.4	9.71E-21	119	127	135	142	148	155	161	166	171	176	181	185	189	3.1378E+02	-9.2838E+01	9.1129E+00	-1	0	-1	0
1098.6	9.82E-21	118	127	134	141	148	154	160	166	171	175	180	184	188	3.0925E+02	-9.2270E+01	8.9711E+00	-1	0	-1	0
1098.8	9.97E-21	117	125	132	139	146	152	158	164	169	174	178	183	187	3.1545E+02	-9.9855E+01	1.0460E+01	-1	0	-1	0
1099.0	1.01E-20	115	123	130	137	143	150	155	161	167	172	176	181	185	3.2237E+02	-1.1911E+02	1.2922E+01	-1	0	-1	0
1099.2	1.05E-20	113	120	127	133	140	146	152	157	162	167	172	176	180	3.1986E+02	-1.1964E+02	1.3349E+01	-1	0	-1	0
1099.4	1.08E-20	112	118	124	131	137	143	149	153	158	163	168	172	176	3.1255E+02	-1.1982E+02	1.3823E+01	-1	0	-1	0
1099.6	1.09E-20	113	120	126	132	138	143	149	153	157	162	166	169	173	2.8719E+02	-9.9474E+01	1.0084E+01	0	-1	0	-1
1099.8	1.11E-20	115	122	128	134	139	144	149	152	156	160	163	167	170	2.5849E+02	-8.6354E+01	8.7569E+00	0	-2	1	-1
1100.0	1.11E-20	116	122	128	134	139	144	148	152	156	159	163	166	168	2.5298E+02	-8.2318E+01	8.0498E+00	0	-2	1	-1
1100.2	1.12E-20	115	121	127	133	138	143	147	152	155	159	163	166	169	2.6838E+02	-8.8979E+01	8.3730E+00	0	-2	1	-1
1100.4	1.12E-20	114	121	127	133	139	144	149	153	157	161	165	168	172	2.7482E+02	-7.9083E+01	8.0918E+00	0	-1	1	-1
1100.6	1.11E-20	114	121	127	133	139	145	150	155	160	164	169	172	176	2.9408E+02	-9.2631E+01	1.0421E+01	0	-1	0	-1
1100.8	1.11E-20	113	120	126	133	139	145	150	155	160	165	170	174	178	3.0801E+02	-1.0340E+02	1.2382E+01	0	-1	0	-1

TABLE 4-I (CONT.)

ν (cm^{-1})	$-\frac{\ell n T}{u}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100 \ell n T}{u}(\theta) / \frac{\ell n T}{u}(296)$ θ (Temperature in Kelvins)													COEFFICIENT			% ERROR			
		350	375	400	425	450	475	500	525	550	575	600	625	650	a_0	a_1	a_2				
1101.0	1.11E-20	113	120	126	133	139	145	150	156	161	166	170	175	179	3.1454E+02	-1.0832E+02	1.3267E+01	0	-1	0	-1
1101.2	1.14E-20	112	118	125	131	137	143	149	154	159	164	169	173	177	3.1777E+02	-1.1299E+02	1.4365E+01	0	-1	0	-1
1101.4	1.17E-20	111	117	124	130	136	141	147	152	157	162	166	170	174	3.1002E+02	-1.0924E+02	1.3933E+01	0	-1	0	-1
1101.6	1.21E-20	111	117	122	128	134	139	144	149	154	159	163	167	171	2.9862E+02	-1.0297E+02	1.3078E+01	0	-1	0	-1
1101.8	1.25E-20	111	116	122	127	132	138	142	147	151	155	159	163	167	2.8371E+02	-9.3709E+01	1.1642E+01	0	-2	1	-1
1102.0	1.27E-20	111	116	122	127	132	137	141	145	149	153	157	160	163	2.6752E+02	-8.2175E+01	9.6464E+00	0	-2	1	-1
1102.2	1.28E-20	111	116	122	127	132	137	141	145	149	153	156	160	163	2.6484E+02	-8.0387E+01	9.3515E+00	0	-2	1	-1
1102.4	1.28E-20	111	116	122	127	132	136	140	145	148	152	156	159	162	2.6179E+02	-7.8618E+01	9.0954E+00	0	-2	2	-1
1102.6	1.29E-20	111	116	121	126	131	135	140	144	147	151	154	157	160	2.5562E+02	-7.4776E+01	8.4991E+00	0	-2	2	-1
1102.8	1.30E-20	111	116	122	126	131	135	139	143	147	150	153	156	159	2.4798E+02	-6.9085E+01	7.4841E+00	0	-2	2	-1
1103.0	1.29E-20	113	118	123	128	133	137	141	145	148	151	154	157	160	2.3969E+02	-6.0473E+01	5.6609E+00	0	-1	1	-1
1103.2	1.28E-20	114	120	126	130	135	139	143	146	149	152	155	158	160	2.2968E+02	-5.0223E+01	3.5042E+00	0	-1	0	-1
1103.4	1.26E-20	115	121	126	131	135	140	143	147	150	153	155	158	160	2.2604E+02	-4.6732E+01	2.7900E+00	0	-1	0	-1
1103.6	1.24E-20	115	121	127	132	136	140	144	147	150	153	156	158	161	2.2332E+02	-4.3742E+01	2.1431E+00	0	-1	0	-1
1103.8	1.22E-20	116	123	128	134	138	143	146	150	153	156	159	162	164	2.3135E+02	-4.7001E+01	2.4041E+00	0	-1	0	-1
1104.0	1.20E-20	117	124	130	135	140	145	149	153	157	160	163	166	169	2.4596E+02	-5.5107E+01	3.5233E+00	0	-1	0	-1
1104.2	1.21E-20	114	120	127	133	138	144	149	154	158	162	166	170	173	2.8469E+02	-8.6565E+01	9.4415E+00	0	-1	0	-1
1104.4	1.23E-20	112	118	124	131	137	142	148	153	158	163	167	171	175	3.0841E+02	-1.0677E+02	1.3343E+01	0	-1	0	-1
1104.6	1.30E-20	109	115	120	126	132	138	143	149	154	158	163	167	171	3.1463E+02	-1.1712E+02	1.5863E+01	0	-1	0	-1
1104.8	1.37E-20	108	113	119	124	130	135	140	145	150	154	159	163	167	3.0148E+02	-1.1055E+02	1.5071E+01	-1	0	-1	0
1105.0	1.43E-20	108	113	118	124	129	134	139	144	148	152	156	160	164	2.9139E+02	-1.0408E+02	1.4038E+01	-1	0	-1	0
1105.2	1.48E-20	111	116	121	125	130	134	138	141	145	148	151	154	157	2.4516E+02	-6.8652E+01	7.6023E+00	-1	0	-1	0
1105.4	1.52E-20	111	116	121	125	130	133	137	140	143	146	149	151	154	2.2515E+02	-5.3866E+01	4.9795E+00	-1	0	-1	0
1105.6	1.54E-20	111	116	120	124	128	132	135	138	141	143	146	148	150	2.1482E+02	-4.8027E+01	4.1562E+00	-1	0	-1	0
1105.8	1.56E-20	111	115	120	124	127	131	134	137	140	142	144	147	149	2.1219E+02	-4.7259E+01	4.1579E+00	-1	0	-1	0
1106.0	1.56E-20	111	116	120	124	127	131	133	136	138	141	143	144	146	1.9542E+02	-3.4487E+01	1.8475E+00	-1	0	-1	0
1106.2	1.56E-20	112	117	121	124	128	131	133	136	138	140	142	144	145	1.8631E+02	-2.7238E+01	5.0054E-01	-1	1	-2	0
1106.4	1.56E-20	112	117	121	125	128	131	134	136	138	140	142	144	146	1.8492E+02	-2.5413E+01	8.1422E-02	-1	1	-2	0
1106.6	1.54E-20	113	118	122	126	129	132	135	138	140	142	144	146	147	1.8923E+02	-2.7280E+01	2.5644E-01	-1	1	-2	0
1106.8	1.52E-20	113	118	123	127	131	134	137	140	142	144	147	148	150	1.9757E+02	-3.1727E+01	8.4247E-01	-1	1	-2	0
1107.0	1.49E-20	114	120	124	129	132	135	139	142	144	147	149	151	153	2.0076E+02	-3.1991E+01	6.4127E-01	-1	0	-1	0
1107.2	1.47E-20	113	119	124	128	133	137	140	144	147	150	152	155	157	2.2596E+02	-5.0391E+01	3.8799E+00	-1	1	-2	0
1107.4	1.47E-20	112	118	123	128	133	137	141	144	148	151	154	157	159	2.3972E+02	-6.0804E+01	5.7563E+00	-1	0	-2	0
1107.6	1.50E-20	110	116	121	125	130	134	139	143	146	150	153	156	159	2.5510E+02	-7.5560E+01	8.7761E+00	-1	1	-2	0
1107.8	1.53E-20	108	113	118	123	127	132	136	140	144	148	152	155	158	2.6595E+02	-8.7075E+01	1.1234E+01	-1	1	-2	0
1108.0	1.57E-20	108	112	117	122	126	131	135	139	143	147	151	154	158	2.7080E+02	-9.2174E+01	1.2319E+01	-1	2	-3	1
1108.2	1.61E-20	106	111	116	121	126	131	135	140	144	148	152	156	160	2.8796E+02	-1.0579E+02	1.4846E+01	-1	2	-3	1
1108.4	1.68E-20	106	110	115	119	124	129	133	138	142	146	150	154	157	2.8145E+02	-1.0298E+02	1.4584E+01	-1	1	-3	0
1108.6	1.76E-20	106	110	115	119	123	128	132	136	139	143	146	150	153	2.6188E+02	-8.9514E+01	1.2313E+01	-1	0	-2	0
1108.8	1.86E-20	107	111	114	118	121	125	128	131	134	136	139	141	144	2.2025E+02	-6.0962E+01	7.5087E+00	0	-1	0	-1
1109.0	1.96E-20	106	109	112	115	118	121	123	126	128	130	132	134	135	1.9190E+02	-4.4118E+01	5.0069E+00	0	-1	0	-1
1109.2	1.99E-20	107	110	113	115	118	120	122	123	125	127	128	129	130	1.6524E+02	-2.4741E+01	1.6074E+00	0	-1	1	-1
1109.4	2.02E-20	108	111	113	115	117	119	119	120	121	121	122	122	123	1.2458E+02	4.3803E+00	-3.4502E+00	0	-2	1	-1
1109.6	1.94E-20	111	114	116	118	119	120	121	122	122	122	123	123	123	1.0895E+02	1.9445E+01	-6.5397E+00	0	-2	1	-1
1109.8	1.85E-20	112	115	118	120	122	123	124	125	125	126	126	126	127	1.1736E+02	1.6054E+01	-6.2732E+00	0	-2	2	-1
1110.0	1.74E-20	114	116	119	122	124	126	127	129	130	131	132	132	133	1.3922E+02	2.9338E+00	-4.3048E+00	0	-1	1	-1
1110.2	1.62E-20	113	118	122	125	128	131	133	135	137	138	140	141	143	1.7032E+02	-1.5062E+01	-1.7023E+00	0	-1	0	-1
1110.4	1.56E-20	113	118	123	127	130	133	135	138	140	142	144	146	148	1.8712E+02	-2.4977E+01	-2.3941E-01	0	-1	0	-1
1110.6	1.53E-20	112	117	122	127	131	135	138	142	145	148	151	153	156	2.2785E+02	-5.4052E+01	4.7980E+00	-1	0	-1	0
1110.8	1.57E-20	109	114	119	124	128	133	137	141	145	148	152	155	158	2.6034E+02	-8.1898E+01	1.0193E+01	-1	0	-1	0
1111.0	1.65E-20	106	110	115	120	125	130	135	140	144	149	153	157	161	2.9523E+02	-1.1176E+02	1.5977E+01	-1	0	-1	0
1111.2	1.75E-20	105	109	113	118	122	127	132	136	140	144	148	152	156	2.8464E+02	-1.0762E+02	1.5679E+01	-1	2	-3	0
1111.4	1.87E-20	104	108	112	116	120	124	128	132	136	139	143	146	149	2.6240E+02	-9.4480E+01	1.3737E+01	-1	3	-4	1
1111.6	1.98E-20	104	107	110	114	118	121	125	128	132	135	138	141	144	2.4667E+02	-8.5673E+01	1.2508E+01	-1	3	-5	1
1111.8	2.06E-20	105	108	111	114	118	121	124	126	129	132	134	136	139	2.1449E+02	-6.1550E+01	8.1878E+00	-1	2	-4	1
1112.0	2.14E-20	105	108	111	114	117	120	122	125	127	129	131	133	135	1.9825E+02	-5.0493E+01	6.3378E+00	-1	2	-3	1
1112.2	2.23E-20	104	107	110	112	115	117	120	122	124	126	128	130	132	1.9213E+02	-4.8727E+01	6.3507E+00	-1	1	-2	0
1112.4	2.32E-20	102	104	107	109	111	114	115	118	120	122	124	126	128	1.9343E+02	-5.4127E+01	7.8354E+00	-1	0	-1	0
1112.6	2.29E-20	105	107	109	112	114	116	118	120	121	123	125	126	127	1.7111E+02	-3.4112E+01	3.8664E+00	0	-1	0	-1
1112.8	2.25E-20	107	110	112	114	116	117	118	119	120	121	121	122	123	1.3235E+02	-2.9580E+00	-1.9590E+00	0	-1	1	-1
1113.0	2.17E-20	109	111	113	115	117	118	119	119	120	120	121	121	121	1.1824E+02	8.8363E+00	-4.2137E+00	0	-2	2	-1
1113.2	2.06E-20	109	113	115	117	119	120	121	122	123	123	124	124	125	1.2567E+02	5.9602E+00	-4.0134E+00	0	-2	1	-1
1113.4	1.97E-20	108	112	114	117	119	120	122	123	125	126	127	128	129	1.4835E+02	-1.0879E+01	-1.0163E+00	0	-2	1	-1
1113.6	1.87E-20	110	114	117	120	122	124	126	128	129	131	132	133	134	1.5573E+02	-1.1782E+01	-1.3954E+00	0	-2	1	-1
1113.8	1.84E-20	109	113	117	120	122	125	127	129	131	133	135	136	138	1.7714E+02	-2.7327E+01	1.3298E+00	0	-1	0	-1
1114.0	1.85E-20	108	112	115	119	122	125	128	131	134	136	138	141	143	2.0715E+02	-4.9973E+01	5.4042E+00	-1	0	-1	0
1114.2	1.85E-20	108	112	116	120	124	127	131	134	137	140	143	146	148	2.3133E+02	-6.6277E+01	8.1113E+00	-1	1	-2	0
1114.4	1.91E-20	106	110	114	118	122	126	130	133	137	140	144	147	150	2.5303E+02	-8.4752E+01	1.1678E+01	-1	2	-3	1
1114.6	1.99E-20	105	109	113	117	120	124	128	132	135	139	142	145	148	2.4903E+02	-8.3584E+01	1.1684E+01	-1	1	-2	0
1114.8	2.12E-20	105	108	111	115	118	122	125	128	131	134	137	139	142	2.2875E+02	-7.1455E+01	9.8700E+00	-1	1	-3	0
1115.0	2.23E-20	106	110	113	116	119	123	125	127	130	132	134	136	138	2.0086E+02	-4.9512E+01	5.8185E+00	-1	2	-4	1
1115.2	2.41E-20	104	106	109	111	114	116	119	121	123	125	127	129	131	1.9169E+02	-4.9420E+01	6.5946E+00	-1	1	-3	1
1115.4	2.57E-20	102	104	106	108	110	112	114	116	118	120	122	124	125	1.8674E+02	-5.1067E+01	7.5163E+00	-1	1	-3	1
1115.6	2.63E-20	106	108	110	112	113	114	115	116	117	118	119	119	120	1.3330E+02	-6.9419E+00	-8.6312E-01	-1	0	-1	0
1115.8	2.73E-20	106	108	110	111	111	112	112	112	112	112	112	112	112	9.7485E+01	1.7310E+01	-4.9033E+00	0	-1	0	-1
1116.0	2.72E-20	109	111	112	112	112	112	111	110	110	109	108	107	106	5.6166E+01	4.9004E+01	-1.0665E+01	-1	0	-2	0
1116.2	2.65E-20	111	113	114	113	113	112	111	109	107	106	104	102	101	1.9604E+01	7.7528E+01	-1.5904E+01	-1	0	-1	0
1116.4	2.52E-20	112	114	115	115	114	113	112	111	109	107	106	104	102	1.8532E+01	8.0223E+01	-1.6608E+01	-1	0	-1	0
1116.6	2.35E-20	113	116	117	118	118	118	117	116	115	114	113	112	110	4.2074E+01	6.7823E+01	-1.5000E+01	-1	0	-1	0
1116.8	2.27E-20	110	113	115	116	118	119	119	119	119	119	119	119	119	9.7322E+01	2.5688E+01	-7.3689E+00	-1	0	-2	0
1117.0	2.20E-20	110	113	115	117	119	120	121	122	122	123	123	124	124	1.1896E+02	1.1275E+01	-4.9989E+00	-1	0	-1	0
1117.2	2.20E-20	109	112	115	117	119	121	123	124	126	127	128	129	130	1.4944E+02	-1.0616E+01	-1.1898E+00	-1	1	-2	0
1117.4	2.16E-20	111	115	119	122	125	128	130	132	134	136	137	139	140	1.7285E+02	-2.0756E+01	-2.3944E-01	-1	2	-4	1
1117.6	2.19E-20	108	112	116	120	123	126	129	132	135	138	140	142	144	2.1312E+02	-5.3440E+01	5.9069E+00	-1	1	-2	0
1117.8	2.25E-20	106	110	114	117	121	124	128	131	134	137	139	142	145	2.2824E+02	-6.7572E+01	8.7653E+00	-1	1	-2	0

TABLE 4-1 (CONT.)

ν (cm^{-1})	$\frac{-\ln T}{u}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100 \ln T}{u}(\theta) / \frac{\ln T}{u}(296)$ θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR
1118.0	2.38E-20	105	108	111	114	117	120	123	126	128	131	133	136	138	2.1214E+02	-6.0386E+01	8.0492E+00	-1 0 -1 0
1118.2	2.53E-20	104	107	109	112	114	117	119	121	123	125	127	128	130	1.8585E+02	-4.4640E+01	5.6916E+00	-1 0 -2 0
1118.4	2.62E-20	106	109	111	113	115	116	118	119	120	121	122	123	124	1.4655E+02	-1.4499E+01	2.1320E-01	-1 0 -2 0
1118.6	2.83E-20	104	106	107	108	109	110	111	112	112	113	113	114	114	1.2349E+02	-4.5074E+00	-7.2379E-01	-1 0 -1 0
1118.8	2.95E-20	103	105	105	106	107	107	108	108	108	108	108	109	109	1.0673E+02	4.4932E+00	-1.9200E+00	-1 0 -2 0
1119.0	3.02E-20	104	105	105	106	106	105	105	105	105	104	104	104	103	8.1452E+01	2.1838E+01	-4.8389E+00	-1 0 -2 0
1119.2	3.04E-20	105	106	106	106	105	104	103	102	101	100	98	97	96	4.1138E+01	5.1419E+01	-1.0063E+01	-1 0 -1 0
1119.4	2.97E-20	106	107	106	106	104	103	101	99	98	96	94	92	90	1.3240E+01	7.1096E+01	-1.3443E+01	0 -1 0 -1
1119.6	2.81E-20	107	108	108	107	106	105	103	101	100	98	96	95	93	1.7816E+01	6.9828E+01	-1.3469E+01	-1 0 -1 0
1119.8	2.68E-20	106	107	108	108	107	107	106	105	104	104	103	102	101	5.6154E+01	4.2944E+01	-8.8697E+00	-1 0 -1 0
1120.0	2.58E-20	106	107	108	109	110	110	110	111	111	111	111	110	110	9.6975E+01	1.5797E+01	-4.4109E+00	-1 0 -1 0
1120.2	2.53E-20	90	91	93	96	99	104	108	112	117	121	125	130	134	3.0532E+02	-1.5325E+02	2.7372E+01	-2 8 -9 3
1120.4	2.42E-20	107	110	113	116	118	120	122	123	125	126	128	129	130	1.6231E+02	-2.2373E+01	1.1628E+00	-1 1 -2 0
1120.6	2.46E-20	107	111	113	116	119	121	123	125	127	129	130	132	133	1.7403E+02	-3.0079E+01	2.4169E+00	-1 1 -2 0
1120.8	2.55E-20	108	111	114	117	119	121	123	125	126	128	129	130	131	1.6092E+02	-1.9865E+01	5.4245E-01	-1 1 -3 1
1121.0	2.65E-20	108	112	114	117	119	121	123	124	126	127	128	130	131	1.5714E+02	-1.6955E+01	1.1825E-02	-1 2 -3 1
1121.2	2.77E-20	108	111	114	116	118	120	122	123	125	126	127	128	129	1.5448E+02	-1.6123E+01	-1.3873E-03	-1 2 -3 1
1121.4	2.93E-20	106	108	111	113	115	117	119	121	122	124	125	126	128	1.6481E+02	-2.7873E+01	2.5718E+00	-1 1 -2 0
1121.6	3.09E-20	106	108	110	112	113	114	115	116	117	118	119	119	120	1.3310E+02	-6.9384E+00	-8.4607E-01	-1 1 -2 0
1121.8	3.25E-20	105	107	108	109	110	111	112	112	113	113	113	113	114	1.1328E+02	4.2603E+00	-2.4244E+00	-1 1 -2 0
1122.0	3.43E-20	104	106	106	107	107	107	107	107	106	106	106	105	105	8.4790E+01	2.0973E+01	-4.8753E+00	-1 0 -2 0
1122.2	3.55E-20	104	105	105	105	104	104	103	102	101	100	99	98	97	5.4928E+01	4.0164E+01	-7.9394E+00	-1 0 -2 0
1122.4	3.62E-20	104	104	104	103	102	101	100	98	97	95	94	93	91	3.3284E+01	5.3358E+01	-9.9485E+00	-1 0 -1 0
1122.6	3.62E-20	104	104	103	102	100	99	97	95	93	91	89	88	86	1.2070E+01	6.6853E+01	-1.2084E+01	0 -1 0 -1
1122.8	3.52E-20	104	104	103	102	100	98	96	94	92	90	87	85	83	-1.8524E+00	7.7021E+01	-1.3874E+01	0 -1 0 -1
1123.0	3.35E-20	103	103	102	100	98	96	94	92	90	87	85	83	81	-2.4100E+00	7.4953E+01	-1.3213E+01	0 -1 0 -1
1123.2	3.15E-20	102	102	101	99	97	95	94	92	90	88	86	84	82	1.0428E+01	6.4073E+01	-1.1118E+01	0 -1 1 -1
1123.4	2.91E-20	103	102	102	101	99	98	96	95	93	92	90	89	87	2.7522E+01	5.3745E+01	-9.5583E+00	0 -2 1 -1
1123.6	2.67E-20	105	106	106	106	105	104	103	102	101	99	98	97	96	3.9962E+01	5.2191E+01	-1.0188E+01	0 -1 0 -1
1123.8	2.59E-20	107	108	108	109	108	108	107	106	105	104	103	102	101	5.4250E+01	4.5657E+01	-9.5059E+00	-1 0 -2 0
1124.0	2.65E-20	103	104	105	106	107	108	109	109	110	110	111	111	112	1.2123E+02	-5.6518E+00	-1.8756E-01	-1 1 -3 1
1124.2	2.80E-20	101	102	103	105	106	107	109	110	111	113	114	115	116	1.5648E+02	-3.3524E+01	4.9746E+00	-1 1 -2 0
1124.4	2.97E-20	104	106	107	109	110	112	113	114	115	116	117	118	119	1.4285E+02	-1.7694E+01	1.4833E+00	-1 2 -4 1
1124.6	3.25E-20	103	105	106	108	109	110	112	113	114	115	116	117	118	1.4427E+02	-2.0334E+01	2.1403E+00	-1 3 -5 2
1124.8	3.54E-20	103	104	105	106	107	108	109	110	110	111	112	112	113	1.2748E+02	-1.0244E+01	6.2440E-01	-1 3 -5 2
1125.0	3.76E-20	103	104	105	106	107	108	109	110	111	112	112	113	114	1.3243E+02	-1.3921E+01	1.2790E+00	-1 2 -3 1
1125.2	4.00E-20	102	103	104	105	106	107	107	108	109	109	110	110	111	1.2551E+02	-1.0565E+01	8.9199E-01	-1 1 -2 0
1125.4	4.26E-20	101	101	102	102	102	102	102	102	102	102	103	103	103	1.0159E+02	2.1347E+00	-7.7086E-01	-1 0 -2 0
1125.6	4.39E-20	102	102	101	101	100	99	98	98	97	96	95	94	94	6.0944E+01	2.9827E+01	-5.4069E+00	-1 0 -2 0
1125.8	4.46E-20	101	101	100	99	97	96	94	93	91	90	88	87	85	3.0063E+01	4.9363E+01	-8.4840E+00	-1 0 -1 0
1126.0	4.41E-20	102	101	99	98	95	93	91	88	86	84	82	79	77	-5.1853E+00	7.3085E+01	-1.2417E+01	0 -1 0 -1
1126.2	4.26E-20	103	102	100	98	95	92	89	86	83	80	77	74	71	-4.0120E+01	9.8763E+01	-1.6957E+01	0 -3 3 -2
1126.4	4.00E-20	104	103	101	99	95	92	88	84	81	77	74	70	67	-6.8057E+01	1.1988E+02	-2.0760E+01	1 -5 7 -4
1126.6	3.61E-20	105	104	102	99	96	93	89	86	82	79	76	72	69	-6.0014E+01	1.1506E+02	-2.0038E+01	0 -3 4 -3
1126.8	3.26E-20	104	103	101	99	96	93	90	87	83	80	77	74	71	-4.9023E+01	1.0674E+02	-1.8537E+01	0 -3 4 -3
1127.0	2.90E-20	106	106	104	102	100	97	94	91	88	85	82	79	76	-4.1648E+01	1.0395E+02	-1.8950E+01	0 -2 2 -2
1127.2	2.75E-20	104	104	103	102	101	99	97	95	93	91	89	87	85	8.1133E+00	6.9938E+01	-1.2651E+01	0 -2 1 -1
1127.4	2.74E-20	101	101	101	100	100	99	99	98	97	97	96	96	95	7.0611E+01	2.2438E+01	-4.0668E+00	-1 0 -1 0
1127.6	2.81E-20	100	100	100	100	101	101	101	101	101	101	101	101	101	9.9630E+01	1.5111E+00	-4.4446E-01	-1 2 -4 1
1127.8	2.99E-20	100	100	100	100	101	101	101	101	101	101	101	101	101	1.0273E+02	-6.4084E-01	-4.9607E-02	-1 3 -6 2
1128.0	3.30E-20	101	101	101	101	102	102	102	102	102	102	102	102	102	1.0010E+02	2.6141E+00	-7.8285E-01	-2 4 -6 3
1128.2	3.66E-20	102	102	102	102	101	101	100	100	99	99	98	97	97	7.0976E+01	2.4127E+01	-4.5985E+00	-2 4 -6 2
1128.4	4.03E-20	102	102	102	102	102	102	102	101	101	101	100	100	99	8.2255E+01	1.6657E+01	-3.3757E+00	-1 2 -4 1
1128.6	4.57E-20	99	99	98	98	97	97	96	96	95	95	94	94	93	7.8744E+01	1.2888E+01	-1.9526E+00	-1 2 -4 1
1128.8	5.03E-20	98	97	96	95	94	93	92	91	90	89	88	87	86	5.5986E+01	2.5846E+01	-3.7940E+00	-1 2 -4 1
1129.0	5.36E-20	98	97	95	94	92	91	89	87	85	84	82	81	80	3.1442E+01	4.1124E+01	-6.1658E+00	-1 1 -2 0
1129.2	5.50E-20	100	98	96	94	92	90	87	85	83	80	78	76	74	-2.3652E+00	6.6376E+01	-1.0678E+01	-1 1 -2 0
1129.4	5.35E-20	103	102	100	97	94	91	87	84	80	77	74	71	68	-5.2936E+01	1.0658E+02	-1.8147E+01	-1 0 -1 0
1129.6	4.97E-20	107	106	104	100	97	92	88	84	79	75	70	66	62	-1.0458E+02	1.4882E+02	-2.6126E+01	0 -1 1 -1
1129.8	4.59E-20	107	106	104	100	96	91	86	81	76	71	66	61	56	-1.3111E+02	1.6716E+02	-2.9231E+01	-1 0 -1 0
1130.0	4.11E-20	109	108	106	102	97	92	87	82	76	71	66	60	55	-1.4911E+02	1.8309E+02	-3.2368E+01	0 -2 2 -2
1130.2	3.60E-20	108	107	105	102	98	94	89	85	80	76	71	67	63	-1.0696E+02	1.5224E+02	-2.6931E+01	-1 0 -1 0
1130.4	3.25E-20	106	106	104	102	99	96	92	89	85	81	78	75	71	-6.4832E+01	1.2222E+02	-2.1735E+01	0 -1 0 -1
1130.6	3.12E-20	104	104	102	100	98	96	93	90	88	85	82	80	77	-2.3920E+01	9.0635E+01	-1.5971E+01	-1 0 -1 0
1130.8	3.14E-20	101	100	99	97	96	94	92	91	89	87	85	84	82	2.3089E+01	5.2319E+01	-8.7479E+00	-1 0 -1 0
1131.0	3.32E-20	95	93	92	91	90	89	88	87	87	86	85	85	84	7.3414E+01	7.0560E+00	2.4083E-01	0 -1 0 -1
1131.2	3.51E-20	92	90	88	87	86	86	86	86	86	86	86	86	86	1.0562E+02	-2.1375E+01	5.8345E+00	0 -1 0 -1
1131.4	3.68E-20	92	89	88	87	86	85	85	85	85	85	85	85	85	1.0105E+02	-1.8570E+01	5.4047E+00	-1 0 -1 0
1131.6	3.93E-20	92	90	88	87	86	85	85	84	84	83	83	83	83	8.9780E+01	-1.0138E+01	3.8962E+00	-1 0 -1 0
1131.8	4.35E-20	92	90	88	86	85	83	82	82	81	80	79	79	78	7.1752E+01	1.5411E+00	2.0188E+00	-1 0 -1 0
1132.0	4.91E-20	92	90	87	85	83	81	79	78	76	75	74	73	72	4.2479E+01	2.1153E+01	-1.2217E+00	-1 1 -3 1
1132.2	5.63E-20	91	87	85	82	80	78	76	75	73	72	71	69	68	4.3024E+01	1.6808E+01	1.6821E-02	-1 1 -3 1
1132.4	6.28E-20	89	85	82	79	77	75	73	72	70	69	68	67	66	4.7293E+01	9.8198E+00	1.7113E+00	-1 2 -4 1
1132.6	6.40E-20	94	91	88	85	82	79	75	72	70	67	65	62	60	-1.8496E+01	6.4753E+01	-8.7849E+00	-1 0 -2 0
1132.8	6.23E-20	100	97	94	90	86	82	78	74	70	66	63	59	55	-7.5653E+01	1.1360E+02	-1.8237E+01	-1 0 -2 0
1133.0	5.75E-20	104	102	99	95	90	85	80	75	70	65	60	56	51	-1.2804E+02	1.5780E+02	-2.6727E+01	-1 0 -1 0
1133.2	5.15E-20	105	104	100	96	91	86	81	76	71	66	61	56	51	-1.3587E+02	1.6543E+02	-2.8302E+01	0 -1 0 -1
1133.4	4.57E-20	105	105	102	98	93	88	83	77	72	67	62	57	52	-1.4198E+02	1.7203E+02	-2.9720E+01	0 -1 1 -1
1133.6	4.07E-20	107	106	103	99	95	90	84	79	74	69	64	59	54	-1.3997E+02	1.7261E+02	-3.0067E+01	0 -3 3 -3
1133.8	3.76E-20	103	102	99	96	92	88	84	80	76	72	68	65	61	-8.1023E+01	1.2330E+02	-2.1228E+01	0 -2 1 -2
1134.0	3.60E-20	100	99	96	93	90	87	84	81	78	75	72	69	66	-3.9550E+01	9.2077E+01	-1.5028E+01	0 -1 0 -1
1134.2	3.60E-20	97	95	93	90	88	85	83	80	78	76	74	72	70	4.6181E-01	5.8616E+01	-8.6293E+00	-1 0 -1 0
1134.4	3.67E-20	95	93	90	88	86	83	81	79	77	75	74	72	71	1.9206E+01	4.1887E+01	-5.3198E+00	-1 0 -2 0
1134.6	3.84E-20	93	90	87	85	83	81	79	78	76	75	73	72	71	3.7617E+01	2.4830E+01	-1.8839E+00	-1 1 -3 1
1134.8	4.04E-20	92	89	86	83	81	79	77	76	74	72	71	70	69	3.6675E+01	2.3129E+01	-1.2979E+00	-1 1 -3 1

TABLE 4-I (CONT.)

ν (cm^{-1})	$\frac{-\ell n T}{u}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100\ell n T}{u}$ (θ) / $\frac{\ell n T}{u}$ (296) θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR
1135.0	4.33E-20	91	87	84	81	79	77	75	73	71	70	68	67	65	3.1854E+01	2.3865E+01	-1.0933E+00	-1 1 -3 1
1135.2	4.75E-20	88	84	81	78	76	73	72	70	68	67	66	64	63	4.1148E+01	1.2561E+01	1.4381E+00	-1 1 -3 1
1135.4	5.06E-20	91	87	84	81	79	76	74	71	69	67	66	64	62	1.6683E+01	3.4545E+01	-2.9254E+00	-1 4 -7 3
1135.6	5.63E-20	89	85	82	78	75	72	70	67	65	63	61	59	58	1.0098E+01	3.4935E+01	-2.4640E+00	-1 4 -7 3
1135.8	6.11E-20	89	84	80	76	73	70	67	64	62	59	57	55	53	-1.0137E+00	4.0348E+01	-3.0927E+00	-1 4 -7 4
1136.0	6.34E-20	90	86	82	78	74	70	67	64	60	58	55	52	50	-2.6346E+01	6.0408E+01	-6.8109E+00	-1 3 -6 3
1136.2	6.35E-20	93	89	85	81	76	72	68	65	61	57	54	51	48	-5.6717E+01	8.6548E+01	-1.1887E+01	-1 2 -4 2
1136.4	6.23E-20	96	92	88	84	79	74	70	65	61	57	53	49	45	-9.0054E+01	1.1502E+02	-1.7393E+01	-1 0 -1 0
1136.6	5.82E-20	99	96	92	88	83	78	73	68	63	58	53	49	44	-1.1758E+02	1.4016E+02	-2.2423E+01	0 -2 2 -2
1136.8	5.36E-20	99	96	92	87	83	78	73	68	63	58	53	49	45	-1.1547E+02	1.3849E+02	-2.2114E+01	0 -3 4 -3
1137.0	4.87E-20	99	95	92	87	82	78	73	68	64	59	55	51	47	-1.0361E+02	1.2950E+02	-2.0492E+01	0 -3 4 -3
1137.2	4.53E-20	97	94	90	86	82	78	73	69	65	62	58	54	51	-7.4204E+01	1.0679E+02	-1.6346E+01	0 -1 1 -1
1137.4	4.33E-20	96	93	89	85	82	78	74	70	67	63	60	57	54	-5.2532E+01	9.0130E+01	-1.3314E+01	-1 0 -1 0
1137.6	4.29E-20	94	90	87	83	80	77	73	70	67	64	62	59	56	-2.8421E+01	7.0109E+01	-9.5006E+00	-1 0 -2 0
1137.8	4.31E-20	93	90	86	83	79	76	73	70	67	64	62	59	57	-2.1436E+01	6.4104E+01	-8.3350E+00	-1 0 -2 0
1138.0	4.33E-20	93	89	86	82	79	76	73	70	67	64	62	59	57	-1.7163E+01	6.0214E+01	-7.5579E+00	-1 0 -1 0
1138.2	4.35E-20	92	89	85	82	78	75	72	69	66	64	61	59	57	-1.5560E+01	5.8119E+01	-7.0785E+00	-1 0 -1 0
1138.4	4.39E-20	92	88	84	81	77	74	71	68	65	62	60	57	55	-2.0259E+01	6.0279E+01	-7.3060E+00	-1 0 -1 0
1138.6	4.47E-20	91	86	82	79	75	72	68	65	63	60	57	55	53	-1.8275E+01	5.6059E+01	-6.2306E+00	-1 0 -2 0
1138.8	4.56E-20	89	85	81	77	73	70	67	64	61	59	56	54	52	-1.2326E+01	4.9326E+01	-4.7590E+00	-1 1 -2 1
1139.0	4.69E-20	88	84	79	75	72	68	65	62	59	57	54	52	50	-1.0101E+01	4.5435E+01	-3.8022E+00	-1 1 -3 1
1139.2	5.01E-20	87	82	77	73	69	66	62	59	56	54	51	49	47	-1.4642E+01	4.5572E+01	-3.4448E+00	-1 1 -4 1
1139.4	5.31E-20	87	81	77	72	68	64	61	57	54	52	49	46	44	-2.3718E+01	5.0902E+01	-4.2275E+00	-1 1 -4 1
1139.6	5.54E-20	87	82	77	73	68	65	61	58	55	52	49	47	45	-2.3049E+01	5.0945E+01	-4.2987E+00	-1 0 -2 0
1139.8	5.76E-20	86	81	76	71	67	63	60	57	54	51	48	46	44	-2.1197E+01	4.7828E+01	-3.5382E+00	-1 0 -1 0
1140.0	5.72E-20	87	82	77	72	68	64	60	57	54	51	48	46	43	-2.7909E+01	5.3956E+01	-4.7643E+00	0 -1 0 -1
1140.2	5.51E-20	88	83	78	74	70	66	62	58	55	52	49	46	43	-3.9203E+01	6.4517E+01	-6.9008E+00	0 -2 1 -2
1140.4	5.27E-20	89	84	79	75	70	66	62	59	55	52	49	46	43	-4.6341E+01	7.1026E+01	-8.2018E+00	0 -1 1 -1
1140.6	5.02E-20	90	85	80	76	71	67	63	59	55	52	49	45	43	-5.3768E+01	7.7493E+01	-9.4655E+00	0 -1 1 -1
1140.8	4.82E-20	90	85	80	76	71	67	63	59	56	53	49	46	44	-4.9020E+01	7.4170E+01	-8.8979E+00	0 -1 1 -1
1141.0	4.69E-20	89	85	80	76	72	68	64	61	57	54	51	49	46	-3.5332E+01	6.4183E+01	-7.1409E+00	0 -1 0 -1
1141.2	4.62E-20	89	85	80	76	72	68	65	61	58	55	52	50	47	-3.0147E+01	6.0797E+01	-6.5930E+00	-1 0 -1 0
1141.4	4.57E-20	90	86	81	77	73	69	65	62	59	56	53	50	47	-3.5510E+01	6.6066E+01	-7.6827E+00	0 -1 0 -1
1141.6	4.49E-20	90	86	82	77	73	69	66	62	59	56	53	50	47	-3.9333E+01	6.9580E+01	-8.3877E+00	0 -1 0 -1
1141.8	4.42E-20	90	86	81	77	73	69	65	62	58	55	52	49	47	-4.1031E+01	7.0173E+01	-8.4147E+00	0 -1 1 -1
1142.0	4.26E-20	90	86	81	77	72	68	64	61	57	54	51	48	45	-4.7339E+01	7.4062E+01	-9.0132E+00	0 -1 1 -1
1142.2	4.08E-20	90	85	80	76	71	67	63	59	55	51	48	45	42	-5.6037E+01	7.9013E+01	-9.7164E+00	0 -2 2 -2
1142.4	4.00E-20	88	83	78	73	69	64	61	57	53	50	47	44	41	-4.3595E+01	6.6513E+01	-7.1066E+00	0 -2 3 -2
1142.6	3.89E-20	87	82	77	72	68	64	60	56	53	50	47	44	41	-4.0434E+01	6.3284E+01	-6.4279E+00	0 -3 3 -3
1142.8	3.95E-20	84	79	74	69	65	61	58	55	52	50	47	45	43	-1.0567E+01	3.7337E+01	-1.3643E+00	0 -1 1 -1
1143.0	4.08E-20	83	77	72	68	64	61	58	55	53	50	49	47	45	7.2841E+00	2.2684E+01	1.4088E+00	-1 1 -2 0
1143.2	4.30E-20	82	76	71	66	63	60	57	54	52	50	49	47	46	2.2873E+01	9.1019E+00	4.0634E+00	-1 1 -3 1
1143.4	4.52E-20	81	75	70	66	62	59	56	54	52	50	48	47	46	2.2359E+01	9.0801E+00	4.1149E+00	-1 0 -2 0
1143.6	4.63E-20	82	76	71	67	63	60	57	55	53	51	49	48	46	1.9013E+01	1.2966E+01	3.2578E+00	-1 0 -1 0
1143.8	4.65E-20	84	78	73	69	65	62	59	56	53	51	49	47	46	5.1756E+00	2.5357E+01	8.0243E-01	0 -1 1 -1
1144.0	4.60E-20	86	81	76	71	67	63	60	57	54	51	49	46	44	-1.7299E+01	4.4918E+01	-3.0184E+00	0 -2 1 -2
1144.2	4.57E-20	87	81	76	72	68	64	60	57	54	51	48	45	43	-2.7389E+01	5.3091E+01	-4.5537E+00	0 -2 2 -2
1144.4	4.45E-20	88	83	78	73	69	65	61	57	54	50	47	44	42	-4.2964E+01	6.6272E+01	-7.0904E+00	0 -2 3 -2
1144.6	4.29E-20	88	83	78	73	69	65	61	57	53	50	47	44	41	-4.6790E+01	6.9302E+01	-7.6523E+00	0 -2 3 -2
1144.8	4.11E-20	87	82	77	72	68	64	60	56	53	50	47	44	42	-3.7079E+01	6.0533E+01	-5.9076E+00	0 -2 2 -2
1145.0	3.85E-20	87	81	76	71	67	63	59	55	52	49	46	43	41	-3.7771E+01	6.0808E+01	-5.6913E+00	0 -2 3 -3
1145.2	3.52E-20	87	82	77	72	67	63	59	56	52	49	46	44	41	-3.7811E+01	6.0580E+01	-5.8573E+00	0 -3 3 -3
1145.4	3.23E-20	87	82	77	73	69	65	61	58	55	52	50	47	45	-2.2527E+01	5.0718E+01	-4.2771E+00	0 -3 3 -3
1145.6	2.99E-20	88	83	78	74	70	67	64	61	58	55	53	51	49	-1.2709E+01	4.5931E+01	-3.7203E+00	0 -2 3 -2
1145.8	2.90E-20	87	82	78	74	70	67	64	62	59	57	55	53	51	4.5029E+00	3.2881E+01	-1.3658E+00	0 -2 2 -2
1146.0	2.92E-20	85	80	76	72	69	66	64	61	59	58	56	54	53	2.2615E+01	1.7674E+01	1.5486E+00	0 -2 2 -2
1146.2	3.01E-20	84	79	74	70	67	65	62	60	58	57	55	54	53	3.3500E+01	7.3332E+00	3.6558E+00	0 -1 1 -1
1146.4	3.14E-20	82	77	73	69	66	63	61	59	57	56	55	54	53	4.3074E+01	1.9172E+00	5.5551E+00	-1 0 -1 0
1146.6	3.24E-20	83	78	73	69	66	63	61	59	57	55	54	53	51	3.2160E+01	6.8677E+00	3.9110E+00	-1 1 -3 1
1146.8	3.33E-20	84	79	74	70	67	64	61	59	57	55	54	52	51	2.3672E+01	1.3957E+01	2.5564E+00	-1 1 -2 1
1147.0	3.38E-20	85	79	75	71	67	64	61	59	57	55	53	51	50	1.4979E+01	2.0922E+01	1.2561E+00	-1 0 -2 0
1147.2	3.37E-20	86	81	76	72	69	65	62	59	57	54	52	50	48	-3.6183E+00	3.6601E+01	-1.7552E+00	-1 0 -1 0
1147.4	3.32E-20	87	82	78	73	69	66	62	59	56	53	51	48	46	-2.1190E+01	5.0823E+01	-4.4254E+00	0 -1 0 -1
1147.6	3.10E-20	90	86	81	77	73	69	65	62	58	55	52	49	46	-4.2358E+01	7.1227E+01	-8.6102E+00	0 -2 2 -2
1147.8	2.88E-20	91	86	82	78	74	70	67	63	60	57	54	52	49	-3.4525E+01	6.7107E+01	-8.0772E+00	0 -3 4 -3
1148.0	2.61E-20	90	86	82	79	75	72	69	66	64	61	59	56	54	-9.8932E+00	5.0111E+01	-5.2044E+00	0 -3 5 -3
1148.2	2.33E-20	91	88	85	81	78	75	73	70	68	66	64	62	60	2.8205E+00	4.4616E+01	-4.6918E+00	0 -3 4 -3
1148.4	2.18E-20	91	88	85	82	79	77	74	72	70	68	66	64	63	1.4841E+01	3.6709E+01	-3.4047E+00	0 -2 1 -1
1148.6	2.14E-20	89	86	83	80	77	75	73	72	70	69	67	66	65	3.8192E+01	1.7134E+01	3.4386E-01	0 -1 0 -1
1148.8	2.16E-20	88	85	82	79	77	75	74	72	71	70	69	68	68	5.7007E+01	2.7549E+00	2.9515E+00	0 -1 0 -1
1149.0	2.20E-20	87	84	81	79	77	76	75	74	73	73	72	72	71	8.0025E+01	-1.4538E+01	6.0532E+00	-1 0 -2 0
1149.2	2.29E-20	88	84	81	79	77	75	74	73	72	71	71	70	70	7.0631E+01	-7.6938E+00	4.8506E+00	0 -1 0 -1
1149.4	2.36E-20	88	84	81	79	77	75	73	72	71	70	69	69	68	6.3048E+01	-2.4695E+00	3.9686E+00	0 -1 1 -1
1149.6	2.38E-20	89	86	83	80	78	76	75	73	72	71	70	69	68	5.1455E+01	8.2340E+00	1.8161E+00	0 -1 1 -1
1149.8	2.34E-20	91	88	85	83	81	78	76	75	73	71	70	69	67	3.2816E+01	2.5169E+01	-1.5637E+00	0 -2 1 -1
1150.0	2.27E-20	93	90	88	85	83	80	78	76	75	73	71	70	68	2.5217E+01	3.3657E+01	-3.4104E+00	0 -2 1 -1
1150.2	2.20E-20	94	91	88	86	84	82	80	78	76	75	73	72	71	3.0649E+01	3.1241E+01	-3.1711E+00	0 -1 1 -1
1150.4	2.13E-20	93	90	88	86	84	82	81	79	78	77	76	75	74	4.7227E+01	1.9157E+01	-1.0468E+00	0 -1 1 -1
1150.6	2.08E-20	92	89	87	85	84	82	81	80	79	78	77	76	76	6.2412E+01	7.1573E+00	1.1747E+00	0 -1 1 -1
1150.8	2.02E-20	92	89	87	86	84	83	82	81	81	80	79	79	79	7.4920E+01	-1.3004E+00	2.5823E+00	0 -1 0 -1
1151.0	1.98E-20	92	90	88	87	86	84	84	83	82	82	81	81	81	7.8763E+01	-2.5481E+00	2.6149E+00	0 -1 0 -1
1151.2	1.97E-20	92	90	89	87	86	85	85	84	83	83	83	82	82	8.4061E+01	-5.6909E+00	3.0810E+00	0 -1 0 -1
1151.4	1.98E-20	92	90	88	87	86	85	84	84	83	83	83	83	82	8.7856E+01	-8.9351E+00	3.7088E+00	0 -1 1 -1
1151.6	1.99E-20	92	90	89	87	86	85	85	84	84	83	83	83	83	8.7497E+01	-8.1249E+00	3.5004E+00	0 -2 2 -1
1151.8	2.02E-20	92	90	88	87	86	85	85	84	84	83	83	83	83	8.9794E+01	-1.0231E+01	3.9227E+00	0 -2 2 -1

TABLE A-1 (CONT.)

ν (cm⁻¹)	$-\frac{1}{u}\frac{\partial \sigma_T}{\partial T}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{10}{u}\frac{\partial \sigma}{\partial T}$ (θ) / $\frac{1}{u}\frac{\partial \sigma}{\partial T}$ (296) — Temperature in K/(Vmax)																	
		350	375	400	425	450	475	500	525	550	575	600	625						
1152.0	2.04E-20	91	89	88	86	86	85	84	84	84	84	84	84	8					
1152.2	2.05E-20	91	89	88	87	86	86	85	85	85	85	85	85	8					
1152.4	2.09E-20	92	90	89	88	87	87	87	87	87	87	87	88	8					
1152.6	2.10E-20	94	93	92	91	91	91	91	91	91	91	91	91	9					
1152.8	2.13E-20	95	94	93	92	92	92	92	92	92	92	92	92	9					
1153.0	2.18E-20	95	94	93	92	92	91	91	91	90	90	90	90	9					
1153.2	2.22E-20	95	94	92	91	90	90	89	88	88	87	87	86	8					
1153.4	2.25E-20	94	93	91	90	89	89	88	87	86	85	84	84	8					
1153.6	2.30E-20	93	91	89	88	87	86	85	84	83	83	82	82	8					
1153.8	2.36E-20	92	89	87	86	84	83	82	82	81	80	80	79	7					
1154.0	2.45E-20	91	89	87	85	83	82	81	80	79	79	79	79	7					
1154.2	2.50E-20	91	89	86	85	83	82	81	80	79	79	78	78	7					
1154.4	2.53E-20	91	89	87	85	84	82	82	81	80	80	79	79	7					
1154.6	2.54E-20	92	89	87	86	84	83	82	82	81	81	80	80	7					
1154.8	2.54E-20	92	90	88	86	85	84	84	83	82	82	82	81	8					
1155.0	2.54E-20	93	91	89	88	87	86	86	85	85	84	84	84	8					
1155.2	2.57E-20	93	91	90	89	88	87	87	86	86	86	86	86	8					
1155.4	2.82E-20	89	87	85	83	83	82	82	82	82	82	82	83	8					
1155.6	3.21E-20	86	83	80	78	77	76	75	75	75	75	75	75	7					
1155.8	3.50E-20	87	83	80	78	77	75	75	74	74	73	73	73	7					
1156.0	3.76E-20	88	84	81	79	77	76	73	72	70	69	68	67	6					
1156.2	3.93E-20	88	84	81	78	75	75	73	70	69	68	65	64	6					
1156.4	3.99E-20	86	84	81	78	75	73	71	69	67	65	64	63	6					
1156.6	3.96E-20	89	85	81	78	76	73	71	69	67	66	64	63	6					
1156.8	3.92E-20	89	85	81	79	76	74	72	70	68	67	66	65	6					
1157.0	3.90E-20	89	85	82	80	77	75	73	72	70	69	68	67	66					
1157.2	3.96E-20	89	86	83	80	78	76	75	73	72	71	70	68	6					
1157.4	4.17E-20	89	85	82	80	78	76	73	73	71	70	69	68	6					
1157.6	4.37E-20	89	85	82	79	77	75	73	72	71	69	68	67	6					
1157.8	4.53E-20	89	85	82	79	77	74	72	71	69	68	66	65	6					
1158.0	4.66E-20	88	84	81	78	75	73	71	70	68	67	66	64	6					
1158.2	4.78E-20	88	84	80	77	75	73	71	69	67	66	65	63	6					
1158.4	4.84E-20	88	84	81	78	75	73	71	69	68	66	65	64	6					
1158.6	4.89E-20	89	85	81	78	76	73	71	69	68	66	65	63	6					
1158.8	4.93E-20	89	86	82	79	77	74	72	70	68	67	65	64	6					
1159.0	4.99E-20	90	86	83	80	77	75	73	71	69	67	66	64	6					
1159.2	5.09E-20	89	86	83	80	77	75	73	71	70	68	67	65	6					
1159.4	5.15E-20	90	87	84	81	79	77	75	73	71	69	68	67	6					
1159.6	5.20E-20	90	87	84	81	79	77	75	73	71	70	68	67	6					
1159.8	5.31E-20	92	88	85	83	80	78	75	73	72	70	68	67	6					
1160.0	5.38E-20	92	89	86	83	81	79	75	74	72	70	69	67	6					
1160.2	5.39E-20	91	88	85	82	80	78	75	74	72	71	69	68	6					
1160.4	5.75E-20	90	87	84	82	80	78	76	75	73	72	71	70	6					
1160.6	5.86E-20	90	86	83	81	79	77	75	74	72	71	70	69	6					
1160.8	5.81E-20	91	87	84	81	78	76	73	71	69	67	65	64	6					
1161.0	5.51E-20	94	90	87	84	81	78	75	72	69	67	64	62	6					
1161.2	5.23E-20	94	91	88	85	81	78	75	72	69	67	64	62	5					
1161.4	5.02E-20	93	90	87	84	81	78	75	72	70	68	65	63	6					
1161.6	4.89E-20	92	89	86	83	80	78	75	73	71	69	67	65	6					
1161.8	4.81E-20	92	89	86	83	80	78	75	73	71	69	67	65	6					
1162.0	4.79E-20	92	88	85	83	80	78	75	73	71	70	68	66	6					
1162.2	4.94E-20	90	87	84	81	78	76	74	72	70	69	67	66	6					
1162.4	5.16E-20	90	86	83	80	78	76	74	72	70	69	67	66	6					
1162.6	5.44E-20	89	85	83	80	78	75	75	74	72	71	71	70	6					
1162.8	5.82E-20	89	85	82	79	77	75	73	71	69	68	68	65	6					
1163.0	6.21E-20	90	86	83	80	77	74	72	70	68	66	65	63	6					
1163.2	6.42E-20	90	86	82	79	76	74	71	69	67	65	64	62	6					
1163.4	6.90E-20	90	86	82	79	76	73	71	68	66	64	62	61	5					
1163.6	7.00E-20	89	85	81	78	75	71	69	66	64	61	59	57	5					
1163.8	6.83E-20	90	86	82	78	75	71	68	66	63	60	58	56	5					
1164.0	6.39E-20	92	88	84	80	77	73	70	67	64	61	59	56	5					
1164.2	5.91E-20	93	89	86	82	78	74	71	68	64	61	59	56	5					
1164.4	5.51E-20	93	90	86	83	80	76	73	70	67	64	62	59	5					
1164.6	5.21E-20	93	90	87	84	81	79	75	73	70	68	66	64	6					
1164.8	5.08E-20	93	90	87	84	82	79	76	74	72	69	67	66	6					
1165.0	5.11E-20	92	89	86	84	81	79	77	75	73	71	70	68	6					
1165.2	5.26E-20	93	90	87	85	82	80	78	77	75	73	72	71	6					
1165.4	5.53E-20	92	89	87	84	82	80	79	77	76	74	73	72	7					
1165.6	5.78E-20	93	90	88	85	83	81	79	77	75	73	72	70	6					
1165.8	6.06E-20	93	90	88	85	82	80	78	76	74	72	70	68	6					
1166.0	6.32E-20	93	90	87	84	82	79	76	74	72	70	68	66	6					
1166.2	6.55E-20	93	90	87	84	81	78	75	73	70	68	66	64	6					
1166.4	6.69E-20	93	89	86	83	80	77	75	72	70	67	65	63	6					
1166.6	6.72E-20	93	89	86	83	80	77	75	72	70	67	65	63	6					
1166.8	6.70E-20	93	89	86	83	80	77	75	72	70	68	66	64	6					
1167.0	6.47E-20	94	91	88	85	82	79	77	74	72	70	68	66	6					
1167.2	6.25E-20	94	91	88	86	83	80	78	75	73	71	69	67	6					
1167.4	5.97E-20	95	92	90	87	84	82	79	77	74	72	70	68	6					
1167.6	5.64E-20	97	95	92	90	87	85	82	80	77	75	73	71	6					
1167.8	5.33E-20	96	96	94	92	89	87	84	82	79	77	75	73	7					
1168.0	5.08E-20	99	97	95	93	91	89	86	84	82	79	77	75	73	2.2320E+00	6.1366E+01	-9.5982E+00	0	-1	0	-1
1168.2	5.00E-20	98	96	94	92	90	88	86	84	82	80	78	76	74	1.2134E+01	5.3146E+01	-8.0326E+00	0	-1	0	-1
1168.4	4.95E-20	97	95	93	91	89	87	85	83	82	80	78	77	75	2.2014E+01	4.4593E+01	-6.3668E+00	-1	0	-1	0
1168.6	4.95E-20	96	95	93	91	89	87	85	84	82	80	79	78	76	3.1215E+01	3.7375E+01	-5.0364E+00	-1	0	-1	0
1168.8	5.03E-20	96	94	92	91	89	87	86	84	83	82	81	79	78	4.2635E+01	2.8925E+01	-3.5357E+00	-1	0	-2	0

TABLE 4-I (CONT.)

ν	$\frac{-hcI}{u}$ $\left(\frac{cm^2}{molecule}\right)$ θ=296K	$\frac{100\,hcI}{u}(\theta) / \frac{hcI}{u}(296)$ θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR
1169.0	5.13E-20	97	95	93	92	90	88	87	85	84	82	81	80	79	3.8300E+01	3.3365E+01	-4.4702E+00	-1 1 -2 0
1169.2	5.37E-20	96	94	92	91	89	87	86	85	83	82	81	80	78	4.3727E+01	2.8155E+01	-3.4836E+00	-1 0 -2 0
1169.4	5.65E-20	95	93	91	89	87	86	84	82	81	80	79	77	76	4.2836E+01	2.6455E+01	-2.8221E+00	-1 0 -2 0
1169.6	5.84E-20	95	93	91	89	87	85	83	82	80	79	77	76	75	3.6347E+01	3.0756E+01	-3.5266E+00	-1 0 -2 0
1169.8	6.00E-20	95	93	91	89	86	84	82	80	78	77	75	73	72	2.1551E+01	4.1211E+01	-5.3251E+00	-1 0 -2 0
1170.0	6.16E-20	95	92	90	88	85	83	81	79	77	75	73	72	70	1.7975E+01	4.2387E+01	-5.3598E+00	-1 0 -1 0
1170.2	6.19E-20	94	92	89	87	85	83	80	78	76	75	73	71	70	1.9689E+01	4.0487E+01	-4.9477E+00	-1 0 -1 0
1170.4	6.05E-20	96	93	91	88	86	84	81	79	77	75	73	72	70	1.1868E+01	4.8093E+01	-6.5138E+00	0 -1 0 -1
1170.6	5.83E-20	96	94	92	90	87	85	83	80	78	76	74	72	71	9.3447E+00	5.1393E+01	-7.2694E+00	0 -2 2 -2
1170.8	5.49E-20	97	95	93	91	89	87	85	83	81	79	77	75	74	1.5191E+01	4.9221E+01	-7.1388E+00	0 -2 2 -2
1171.0	5.18E-20	97	95	93	91	90	88	86	84	83	81	80	78	77	3.1045E+01	3.8477E+01	-5.3476E+00	0 -1 1 -1
1171.2	4.84E-20	99	97	96	94	92	91	89	87	86	84	83	81	80	2.8200E+01	4.4258E+01	-6.8097E+00	0 -1 1 -1
1171.4	4.59E-20	100	99	98	96	95	93	91	90	88	86	85	83	82	2.3294E+01	5.1882E+01	-8.3996E+00	0 -1 0 -1
1171.6	4.41E-20	101	100	99	98	97	95	94	92	91	89	88	86	85	3.1818E+01	4.7086E+01	-7.9636E+00	0 -1 0 -1
1171.8	4.32E-20	101	101	100	98	97	96	94	93	91	90	88	87	86	3.3443E+01	4.6470E+01	-7.9237E+00	0 -1 0 -1
1172.0	4.29E-20	101	100	100	98	97	96	94	93	92	90	89	87	86	3.5804E+01	4.4832E+01	-7.6456E+00	0 -1 0 -1
1172.2	4.34E-20	100	99	98	97	96	95	93	92	91	90	88	87	86	4.5044E+01	3.6076E+01	-5.8633E+00	-1 0 -1 0
1172.4	4.41E-20	99	98	97	96	95	94	93	92	91	90	89	88	87	5.0858E+01	3.1124E+01	-4.9870E+00	-1 0 -1 0
1172.6	4.52E-20	99	98	97	96	95	94	92	91	90	89	88	87	86	5.1756E+01	2.9779E+01	-4.5877E+00	-1 0 -2 0
1172.8	4.63E-20	99	98	97	96	95	93	92	91	89	88	87	86	85	4.3580E+01	3.5559E+01	-5.5821E+00	-1 0 -2 0
1173.0	4.76E-20	99	98	97	95	94	93	91	90	88	87	85	84	83	3.6641E+01	4.0854E+01	-6.3047E+00	-1 0 -2 0
1173.2	4.92E-20	98	97	95	94	92	91	89	88	86	85	83	82	81	3.6143E+01	3.8172E+01	-5.7040E+00	-1 0 -2 0
1173.4	5.02E-20	98	96	95	93	92	90	88	87	85	84	83	81	80	3.7281E+01	3.6286E+01	-5.2456E+00	-1 1 -2 0
1173.6	5.04E-20	98	97	95	94	92	90	89	87	85	84	82	81	79	2.8459E+01	4.3746E+01	-6.6806E+00	-1 1 -2 0
1173.8	4.97E-20	100	99	98	96	94	92	90	88	86	84	83	81	79	1.5580E+01	5.5717E+01	-9.0956E+00	-1 0 -2 0
1174.0	4.84E-20	102	101	99	98	96	93	91	89	87	85	82	80	78	-1.3283E-01	6.9535E+01	-1.1809E+01	-1 0 -1 0
1174.2	4.63E-20	102	102	100	99	97	95	92	90	88	86	83	81	79	-3.1395E+00	7.3253E+01	-1.2646E+01	0 -1 1 -1
1174.4	4.39E-20	102	102	100	99	97	96	94	92	90	88	86	85	83	1.4679E+01	6.0858E+01	-1.0538E+01	0 -2 2 -2
1174.6	4.19E-20	102	101	101	99	98	96	95	93	92	90	89	87	86	2.7208E+01	5.2295E+01	-9.1816E+00	0 -2 2 -2
1174.8	3.90E-20	103	104	103	102	102	100	99	98	97	95	94	93	92	4.0078E+01	4.7382E+01	-8.7749E+00	0 -2 1 -1
1175.0	3.71E-20	105	106	106	106	105	104	103	102	101	99	98	97	96	4.1630E+01	5.0790E+01	-9.9197E+00	0 -1 0 -1
1175.2	3.64E-20	106	107	108	107	106	106	104	103	102	100	99	98	96	3.5151E+01	5.7577E+01	-1.1361E+01	0 -1 0 -1
1175.4	3.74E-20	103	104	104	103	103	102	101	100	99	98	97	96	95	5.3539E+01	3.9691E+01	-7.3819E+00	-1 0 -1 0
1175.6	3.74E-20	104	104	104	104	103	102	102	101	100	99	98	97	96	5.1343E+01	4.1369E+01	-7.9707E+00	-1 1 -2 0
1175.8	3.84E-20	103	103	103	103	102	101	100	99	98	97	96	95	94	5.2187E+01	3.8993E+01	-7.3543E+00	-1 1 -2 0
1176.0	4.03E-20	101	100	100	99	98	97	97	96	95	94	93	92	91	5.9259E+01	2.8883E+01	-4.9799E+00	-1 1 -3 1
1176.2	4.18E-20	100	99	99	98	97	97	96	95	94	93	92	92	91	6.3139E+01	2.4673E+01	-4.0735E+00	-1 2 -4 1
1176.4	4.36E-20	98	98	97	96	95	94	94	93	92	92	91	90	90	6.9333E+01	1.7258E+01	-2.4214E+00	-1 2 -4 1
1176.6	4.56E-20	98	97	96	95	94	93	91	90	89	88	87	86	85	4.9029E+01	3.0572E+01	-4.5835E+00	-1 1 -3 1
1176.8	4.63E-20	99	98	97	96	94	92	91	89	87	86	84	83	82	2.8625E+01	4.6082E+01	-7.3865E+00	-1 0 -1 0
1177.0	4.56E-20	101	100	99	97	95	93	91	89	87	85	83	82	80	1.0639E+01	6.0956E+01	-1.0213E+01	0 -1 0 -1
1177.2	4.33E-20	103	102	101	99	97	95	93	91	88	86	84	82	80	-5.2489E+00	7.5859E+01	-1.3233E+01	0 -3 3 -2
1177.4	4.03E-20	105	105	104	102	101	99	97	94	92	90	88	86	84	-2.8261E+00	7.8235E+01	-1.4148E+01	0 -3 4 -3
1177.6	3.74E-20	104	104	104	103	101	100	98	96	95	93	91	90	88	2.0402E+01	6.1702E+01	-1.1298E+01	0 -4 5 -3
1177.8	3.45E-20	104	105	104	103	102	101	99	97	96	94	92	91	89	2.2225E+01	6.1368E+01	-1.1351E+01	0 -3 3 -2
1178.0	3.13E-20	107	109	109	108	108	107	105	104	102	101	99	98	96	2.7453E+01	6.4827E+01	-1.2832E+01	0 -2 2 -2
1178.2	2.94E-20	109	110	111	111	111	110	110	109	107	106	105	104	103	4.3812E+01	5.7001E+01	-1.1949E+01	0 -1 0 -1
1178.4	2.90E-20	106	107	108	109	109	109	109	109	108	108	107	107	106	7.8221E+01	2.8774E+01	-6.6100E+00	-1 0 -1 0
1178.6	2.90E-20	105	106	107	107	108	108	108	108	108	108	108	107	107	9.1787E+01	1.6879E+01	-4.2767E+00	-1 0 -1 0
1178.8	2.93E-20	104	105	105	106	106	107	107	107	107	107	107	107	107	9.8000E+01	1.0457E+01	-2.9199E+00	-1 1 -2 0
1179.0	2.99E-20	104	105	105	106	106	106	106	106	106	106	106	106	105	9.1593E+01	1.5051E+01	-3.7184E+00	-1 2 -3 1
1179.2	3.08E-20	103	104	104	105	105	105	105	105	104	104	104	104	104	9.0080E+01	1.4333E+01	-3.8732E+00	-1 2 -4 1
1179.4	3.16E-20	103	103	104	104	104	104	104	104	104	103	103	103	103	8.9815E+01	1.3404E+01	-3.6754E+00	-1 2 -4 1
1179.6	3.27E-20	102	102	102	102	102	102	102	102	102	102	101	101	101	8.9380E+01	1.1783E+01	-2.5574E+00	-1 2 -4 1
1179.8	3.37E-20	102	102	102	102	102	102	101	101	101	100	100	100	99	8.3748E+01	1.5271E+01	-3.0962E+00	-1 1 -3 1
1180.0	3.45E-20	101	101	101	101	101	100	100	100	99	99	99	98	98	8.2250E+01	1.4733E+01	-2.8058E+00	-1 1 -3 1
1180.2	3.44E-20	103	103	103	103	102	102	101	101	100	99	99	98	97	6.7832E+01	2.7697E+01	-5.3797E+00	-1 1 -2 0
1180.4	3.35E-20	105	106	106	106	105	104	103	102	101	100	98	97	96	4.2833E+01	4.9816E+01	-9.7368E+00	-1 1 -2 0
1180.6	3.20E-20	108	109	109	109	108	107	106	104	103	101	99	98	96	2.4966E+01	6.7209E+01	-1.3320E+01	0 -1 0 -1
1180.8	3.05E-20	108	110	110	109	109	107	106	104	103	101	99	98	96	1.8641E+01	7.2580E+01	-1.4355E+01	0 -1 0 -1
1181.0	2.90E-20	107	108	109	108	108	107	105	104	103	101	100	99	97	3.2144E+01	6.1329E+01	-1.2208E+01	0 -2 1 -1
1181.2	2.69E-20	108	109	110	110	110	109	109	108	107	106	104	103	102	4.8418E+01	5.2109E+01	-1.0905E+01	0 -2 1 -1
1181.4	2.48E-20	109	111	112	113	113	113	113	113	113	112	112	111	110	7.4928E+01	3.5745E+01	-8.6799E+00	0 -1 0 -1
1181.6	2.42E-20	107	109	110	111	112	113	114	114	114	115	115	115	115	1.0832E+02	1.0727E+01	-3.9044E+00	-1 0 -2 0
1181.8	2.45E-20	104	106	107	108	110	111	112	112	113	114	115	115	116	1.3877E+02	-9.7743E+00	1.9761E-01	-1 1 -2 0
1182.0	2.54E-20	101	102	103	104	106	107	108	109	111	112	113	114	115	1.5411E+02	-3.2442E+01	4.8620E+00	-1 2 -3 1
1182.2	2.66E-20	99	100	101	102	104	105	105	108	109	110	111	113	114	1.5877E+02	-3.8460E+01	6.2350E+00	-1 3 -4 1
1182.4	2.80E-20	99	100	101	102	102	103	104	105	106	107	108	109	110	1.4330E+02	-2.8398E+01	4.6124E+00	-1 3 -4 1
1182.6	2.99E-20	99	99	99	100	101	101	102	103	104	105	105	106	107	1.3648E+02	-2.5834E+01	4.4502E+00	-1 2 -4 1
1182.8	3.15E-20	97	97	98	98	99	100	101	102	103	104	105	106	106	1.4510E+02	-3.4378E+01	6.2240E+00	-1 2 -3 1
1183.0	3.30E-20	97	97	97	97	98	98	99	99	100	100	101	102	102	1.2848E+02	-2.3755E+01	4.5365E+00	-1 1 -2 0
1183.2	3.33E-20	99	99	99	99	99	99	99	98	98	98	98	98	98	9.6151E+01	1.8529E+00	-2.1125E-01	-1 1 -2 0
1183.4	3.29E-20	102	102	101	101	100	99	98	98	97	96	95	94	93	6.0031E+01	3.0547E+01	-5.5398E+00	-1 1 -2 0
1183.6	3.13E-20	105	106	105	105	103	102	101	99	98	96	94	93	91	2.4916E+01	6.1204E+01	-1.1538E+01	-1 0 -1 0
1183.8	2.97E-20	106	107	107	106	105	103	102	100	98	97	95	93	91	1.6981E+01	6.8977E+01	-1.3143E+01	0 -1 1 -1
1184.0	2.71E-20	109	110	111	110	109	108	107	105	103	102	100	98	96	1.6493E+01	7.5167E+01	-1.4929E+01	0 -3 3 -2
1184.2	2.50E-20	110	112	112	112	111	110	108	106	105	103	101	99	97	1.0045E+01	8.2153E+01	-1.6436E+01	0 -3 4 -3
1184.4	2.34E-20	109	111	112	112	111	110	109	107	106	104	103	101	100	2.5995E+01	7.0197E+01	-1.4294E+01	0 -3 3 -2
1184.6	2.20E-20	107	109	110	110	111	111	110	110	109	109	108	107	107	7.0578E+01	3.6553E+01	-8.2418E+00	0 -2 1 -1
1184.8	2.09E-20	108	110	111	112	112	113	113	112	112	112	111	111	110	7.9701E+01	3.2102E+01	-7.7237E+00	0 -1 0 -1
1185.0	2.06E-20	105	107	108	110	110	111	112	112	112	113	113	113	113	1.1146E+02	5.7555E+00	-2.7078E+00	-1 0 -1 0
1185.2	2.06E-20	104	105	107	108	109	109	110	111	111	112	112	113	113	1.2856E+02	-3.3773E+00	-8.9201E-01	-1 1 -2 0
1185.4	2.09E-20	102	103	105	106	107	108	109	110	110	111	111	113	113	1.3412E+02	-1.5863E+01	1.7057E+00	-1 2 -4 1
1185.6	2.16E-20	100	101	102	104	105	106	107	108	109	110	111	112	113	1.4751E+02	-2.8483E+01	4.2687E+00	-1 3 -5 1
1185.8	2.25E-20	98	99	100	101	102	103	104	106	107	108	109	110	111	1.5462E+02	-3.7621E+01	6.3501E+00	-2 4 -6 2

TABLE 4-1 (CONT.)

ν (cm⁻¹)	$-\frac{\Delta_T}{u}$ ($\frac{cm^2}{molecule}$) 0-296K	$\frac{100\,\Delta_T}{u}$ (θ) / $\frac{\Delta_T}{u}$ (296) θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR			
1186.0	2.45E-20	94	93	93	94	95	96	97	99	100	102	103	104	106	1.6728E+02	-5.6183E+01	1.9735E+01	-2	4	-6	2
1186.2	2.92E-20	96	95	95	95	96	96	97	98	99	100	100	101	102	1.4028E+02	-3.4997E+01	6.8298E+00	-1	3	-5	2
1186.4	2.61E-20	95	95	94	94	94	95	95	96	96	97	97	98	98	1.2430E+02	-2.6207E+01	5.4524E+00	-1	2	-4	1
1186.6	2.66E-20	96	96	95	95	95	95	95	95	96	96	96	96	97	1.1387E+02	-1.6379E+01	3.6326E+00	-1	2	-4	1
1186.8	2.68E-20	97	96	96	96	96	95	95	95	95	95	95	95	96	1.0269E+02	-7.1972E+00	1.8979E+00	-1	2	-3	1
1187.0	2.70E-20	98	97	97	97	96	96	95	95	95	95	94	94	94	8.8708E+01	4.0142E+00	-1.9885E-01	-1	1	-2	0
1187.2	2.64E-20	100	100	100	99	99	98	98	97	96	96	95	94	94	7.1295E+01	2.8416E+01	-3.5283E+00	-1	0	-2	0
1187.4	2.51E-20	104	104	104	104	103	102	101	100	99	98	97	96	95	4.8283E+01	4.3298E+01	-8.2583E+00	-1	0	-1	0
1187.6	2.39E-20	107	107	108	107	106	105	104	103	101	100	98	97	95	3.0567E+01	4.0829E+01	-1.1922E+01	0	-1	0	-1
1187.8	2.25E-20	109	110	111	110	109	108	107	105	104	102	101	99	97	2.2120E+01	7.1133E+01	-1.4232E+01	0	-1	0	-1
1188.0	2.11E-20	110	111	112	112	111	110	109	108	106	105	103	102	100	2.5264E+01	7.1227E+01	-1.4535E+01	0	-1	0	-1
1188.2	2.05E-20	107	108	109	109	109	109	108	108	107	106	105	104	104	6.0370E+01	4.2267E+01	-9.0389E+00	-1	0	-1	0
1188.4	2.04E-20	104	105	105	106	106	106	106	106	106	106	106	105	105	9.1873E+01	1.4402E+01	-3.5908E+00	-1	1	-2	0
1188.6	2.03E-20	101	102	103	103	104	104	104	104	105	105	105	105	105	1.2748E+02	-2.7324E+01	5.6236E+00	-1	2	-4	1
1188.8	2.04E-20	98	100	100	100	101	101	102	102	103	103	104	104	104	1.5257E+02	-1.4078E+01	2.4541E+00	-1	2	-3	0
1189.0	2.09E-20	98	98	98	98	98	99	99	100	101	101	102	102	103	1.2758E+02	-2.1992E+01	4.0929E+00	-1	1	-3	0
1189.2	2.17E-20	96	96	96	96	97	97	98	98	99	100	100	101	102	1.3243E+02	-2.8821E+01	5.4531E+00	-1	2	-4	1
1189.4	2.25E-20	96	96	96	96	96	96	97	97	97	98	98	99	99	1.2158E+02	-2.0840E+01	4.2781E+00	-1	2	-4	1
1189.6	2.33E-20	96	96	95	95	95	95	95	96	96	96	96	97	97	1.1348E+02	-1.5682E+01	3.4604E+00	-1	2	-4	1
1189.8	2.40E-20	97	97	96	96	95	95	95	95	94	94	94	94	94	9.5340E+01	-2.0958E+00	1.0286E+00	-1	1	-3	1
1190.0	2.44E-20	98	98	97	97	96	96	96	95	95	95	94	94	94	8.7158E+01	5.3724E+00	-4.6438E-01	-1	1	-2	0
1190.2	2.43E-20	99	98	98	98	97	97	96	96	96	95	95	95	94	8.3943E+01	8.9839E+00	-1.2524E+00	-1	0	-2	0
1190.4	2.35E-20	102	102	101	101	100	99	99	98	97	96	95	94	93	5.9025E+01	3.1589E+01	-5.7363E+00	0	-1	0	-1
1190.6	2.24E-20	105	105	105	104	103	101	100	99	97	96	94	93	91	2.8721E+01	5.7412E+01	-1.0749E+01	0	-2	2	-2
1190.8	2.12E-20	108	107	106	106	104	102	101	99	97	95	93	91	89	6.9493E+00	7.9511E+01	-1.4199E+01	0	-3	3	-2
1191.0	2.01E-20	106	107	106	106	105	103	102	100	98	97	95	93	92	2.0609E+01	6.9971E+01	-1.2571E+01	0	-2	2	-2
1191.2	1.92E-20	105	105	105	105	104	103	102	101	100	99	98	96	95	4.4139E+01	4.7720E+01	-9.2309E+00	0	-2	1	-1
1191.4	1.86E-20	103	103	103	103	103	103	102	101	101	100	100	99	99	7.2342E+01	2.5109E+01	-5.0089E+00	0	-1	0	-1
1191.6	1.85E-20	102	102	102	102	102	102	102	101	101	101	100	100	100	8.3663E+01	1.5769E+01	-3.2351E+00	-1	0	-1	0
1191.8	1.84E-20	101	101	101	101	101	101	101	101	101	101	101	101	101	9.7487E+01	4.3777E+00	-1.0756E+00	-1	1	-2	0
1192.0	1.84E-20	99	100	100	100	101	101	101	102	102	103	103	103	104	1.1728E+02	-1.1313E+01	1.8345E+00	-1	1	-3	0
1192.2	1.85E-20	99	100	100	100	101	102	102	103	103	104	104	105	105	1.2386E+02	-1.5827E+01	2.5941E+00	-1	1	-2	0
1192.4	1.88E-20	99	100	100	100	101	101	102	102	102	103	103	104	104	1.1855E+02	-1.2205E+01	1.9870E+00	-1	1	-2	0
1192.6	1.92E-20	100	100	100	100	101	101	101	101	101	101	101	101	101	1.0880E+02	6.8855E-01	-2.7414E-01	-1	1	-2	0
1192.8	1.94E-20	101	101	101	101	101	101	102	100	100	100	99	99	99	8.7805E+01	1.8773E+01	-2.1202E+00	-1	1	-2	0
1193.0	1.95E-20	101	101	101	101	101	101	100	100	99	99	99	98	98	7.9510E+01	1.7299E+01	-3.3247E+00	-1	1	-2	0
1193.2	1.96E-20	103	103	103	103	102	102	101	100	99	99	98	97	96	6.3688E+01	3.0610E+01	-5.8814E+00	-1	1	-2	0
1193.4	1.95E-20	103	104	104	103	103	102	101	100	100	99	98	97	96	5.7209E+01	3.6336E+01	-7.0806E+00	-1	1	-2	0
1193.6	1.92E-20	104	105	105	104	104	103	102	101	100	98	97	96	95	4.5401E+01	4.4151E+01	-8.8944E+00	-1	0	-1	0
1193.8	1.89E-20	106	106	106	105	104	103	102	100	99	97	96	94	93	2.7708E+01	6.0263E+01	-1.1512E+01	0	-1	0	-1
1194.0	1.88E-20	104	105	104	104	103	102	100	99	97	96	95	93	92	3.4247E+01	5.3218E+01	-9.9915E+00	0	-1	0	-1
1194.2	1.85E-20	105	105	105	104	103	102	101	99	98	96	95	93	92	3.2157E+01	5.5257E+01	-1.0412E+01	0	-1	1	-1
1194.4	1.84E-20	105	106	106	106	105	104	102	101	100	98	97	95	94	3.1838E+01	5.8369E+01	-1.1232E+01	0	-2	1	-1
1194.6	1.76E-20	106	107	107	107	106	105	104	102	101	99	98	96	95	2.9539E+01	6.1164E+01	-1.1932E+01	0	-2	2	-2
1194.8	1.74E-20	107	108	108	107	106	105	104	102	101	99	98	96	95	2.8420E+01	6.2290E+01	-1.2166E+01	0	-2	1	-1
1195.0	1.74E-20	106	107	107	106	106	105	104	102	101	100	98	97	96	3.4017E+01	5.5882E+01	-1.0935E+01	0	-1	1	-1
1195.2	1.74E-20	105	106	106	106	105	104	103	102	101	100	99	98	97	4.7933E+01	4.6118E+01	-9.0892E+00	0	-1	0	-1
1195.4	1.74E-20	105	106	106	106	105	104	104	103	102	101	100	99	97	5.8870E+01	4.4070E+01	-8.7401E+00	-1	0	-1	0
1195.6	1.75E-20	105	106	106	106	105	105	104	103	102	101	100	99	98	5.4535E+01	4.1723E+01	-8.3669E+00	-1	0	-1	0
1195.8	1.76E-20	105	106	106	106	106	105	104	104	103	102	101	100	99	5.6692E+01	4.0399E+01	-8.1636E+00	-1	0	-1	0
1196.0	1.76E-20	106	107	107	107	107	106	105	104	103	102	101	100	99	4.8790E+01	4.7836E+01	-9.6725E+00	-1	0	-1	0
1196.2	1.77E-20	105	107	107	107	107	106	105	105	104	103	102	100	99	5.1341E+01	4.5985E+01	-9.3483E+00	-1	0	-1	0
1196.4	1.78E-20	105	107	108	108	107	106	105	105	104	103	102	100	99	4.8998E+01	4.8068E+01	-9.7596E+00	-1	0	-1	0
1196.6	1.77E-20	106	107	108	108	107	107	106	105	104	102	101	100	99	4.6624E+01	4.9988E+01	-1.0120E+01	-1	0	-1	0
1196.8	1.75E-20	108	109	109	110	108	108	106	105	104	103	101	100	98	3.4784E+01	6.0449E+01	-1.2179E+01	0	-1	1	-1
1197.0	1.74E-20	108	109	110	109	109	107	106	105	103	102	100	99	97	2.8418E+01	6.5238E+01	-1.3839E+01	0	-2	1	-1
1197.2	1.71E-20	108	109	109	109	108	107	106	105	103	102	100	98	97	2.7302E+01	6.5549E+01	-1.3950E+01	0	-2	2	-2
1197.4	1.68E-20	109	110	110	110	109	108	107	106	104	103	101	100	98	2.7402E+01	6.6834E+01	-1.3429E+01	0	-3	3	-2
1197.6	1.64E-20	107	109	109	110	109	107	106	105	103	102	100	99	97	3.1277E+01	6.2535E+01	-1.2489E+01	0	-3	3	-2
1197.8	1.62E-20	107	108	108	108	108	107	105	104	103	102	101	99	98	3.7540E+01	5.7294E+01	-1.1487E+01	0	-3	3	-2
1198.0	1.60E-20	106	107	107	107	107	106	105	105	104	103	102	101	100	5.2009E+01	4.5541E+01	-9.2753E+00	0	-3	3	-2
1198.2	1.59E-20	105	106	106	106	106	105	105	104	103	103	102	101	100	5.9913E+01	3.8667E+01	-7.9332E+00	0	-2	1	-1
1198.4	1.59E-20	104	105	105	105	105	105	105	104	103	103	102	102	101	7.0576E+01	2.9632E+01	-6.1930E+00	0	-1	0	-1
1198.6	1.59E-20	104	104	105	105	105	105	104	104	104	103	103	103	102	8.0131E+01	2.1915E+01	-4.7481E+00	-1	0	-1	0
1198.8	1.59E-20	104	105	105	105	105	105	105	104	104	104	103	103	102	7.8746E+01	2.3377E+01	-5.0575E+00	-1	0	-2	0
1199.0	1.59E-20	104	105	105	106	105	105	105	104	104	104	103	103	102	7.5818E+01	2.5845E+01	-5.5314E+00	-1	1	-3	0
1199.2	1.60E-20	104	105	106	106	106	105	105	104	104	103	103	102	102	7.2806E+01	2.8227E+01	-5.9711E+00	-1	2	-3	1
1199.4	1.60E-20	104	105	106	106	106	105	105	104	104	103	102	102	101	6.8591E+01	3.1570E+01	-6.5992E+00	-1	2	-4	1
1199.6	1.60E-20	105	106	107	107	106	106	105	105	104	103	102	101	101	6.1127E+01	3.8031E+01	-7.8911E+00	-1	2	-4	1
1199.8	1.58E-20	107	108	109	109	108	108	107	106	105	104	103	101	100	4.6977E+01	5.1101E+01	-1.0480E+01	-1	1	-2	0
1200.0	1.57E-20	107	109	109	109	109	108	107	106	105	103	102	101	100	4.1852E+01	5.5744E+01	-1.1257E+01	-1	0	-1	0
1200.2	1.54E-20	107	109	109	109	109	109	107	106	105	104	103	102	101	4.4590E+01	5.3869E+01	-1.1891E+01	0	-1	0	-1
1200.4	1.49E-20	108	110	110	111	110	110	109	108	107	106	105	104	103	4.7402E+01	5.3502E+01	-1.1228E+01	0	-1	0	-1
1200.6	1.43E-20	111	112	113	113	113	112	112	111	109	108	107	106	105	4.1805E+01	6.1797E+01	-1.3123E+01	-1	0	-1	0
1200.8	1.33E-20	113	116	116	116	119	119	119	117	116	115	114	112	111	4.1718E+01	6.8943E+01	-1.5301E+01	-1	0	-1	0
1201.0	1.29E-20	113	116	118	119	120	120	120	119	118	118	117	116	115	5.7344E+01	5.8704E+01	-1.3639E+01	-1	0	-1	0
1201.2	1.26E-20	114	117	120	121	122	122	122	122	121	120	120	119	118	6.5897E+01	5.4557E+01	-1.3161E+01	-1	0	-1	0
1201.4	1.26E-20	111	114	119	118	119	120	120	121	121	121	121	121	121	9.5767E+01	2.9894E+01	-8.2420E+00	-1	1	-2	0
1201.6	1.26E-20	110	112	115	116	118	119	120	120	121	121	121	122	122	1.1295E+02	1.4341E+01	-3.3791E+00	-1	1	-3	0
1201.8	1.26E-20	109	112	115	116	118	119	120	120	121	121	122	122	122	1.1601E+02	1.2043E+01	-4.9678E+00	-1	1	-3	0
1202.0	1.28E-20	109	112	114	116	117	119	119	120	120	120	121	121	121	1.1409E+02	1.2583E+01	-4.9503E+00	-1	1	-2	0
1202.2	1.31E-20	109	111	114	115	116	117	118	119	119	119	120	120	120	1.1123E+02	1.3819E+01	-5.0746E+00	-1	1	-2	0
1202.4	1.34E-20	109	112	114	115	116	117	118	118	119	119	119	119	119	1.0814E+02	1.7442E+01	-5.7004E+00	-1	1	-2	0
1202.6	1.37E-20	108	111	113	114	115	116	116	117	117	117	117	117	117	1.0412E+02	1.7401E+01	-5.5295E+00	-1	1	-2	0
1202.8	1.37E-20	110	113	115	116	117	117	118	118	118	118	118	117	117	9.1838E+01	2.8871E+01	-7.8306E+00	-1	1	-3	1

TABLE 4-I (CONT.)

ν (cm^{-1})	$\frac{-k_T}{u}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100\,k_T}{u}(\theta) / \frac{k_T}{u}(296)$ — θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR
1203.0	1.34E-20	113	116	119	120	120	121	120	120	119	119	118	117	116	6.3193E+01	5.4859E+01	-1.3013E+01	-1 1 -2 0
1203.2	1.33E-20	114	118	119	120	121	121	120	119	118	117	116	115	114	4.4880E+01	6.9103E+01	-1.5625E+01	-1 0 -1 0
1203.4	1.32E-20	115	119	121	121	121	121	120	119	117	116	114	113	111	2.5307E+01	8.4473E+01	-1.8460E+01	-1 0 -1 0
1203.6	1.29E-20	117	121	123	124	123	123	122	120	119	117	115	114	112	1.5434E+01	9.4614E+01	-2.0596E+01	-1 0 -1 0
1203.8	1.26E-20	116	120	122	123	123	122	122	121	120	118	117	115	114	3.1806E+01	8.1515E+01	-1.8154E+01	-1 0 -1 0
1204.0	1.22E-20	115	118	121	122	122	123	122	122	121	120	119	118	117	5.3116E+01	6.5206E+01	-1.5193E+01	-1 0 -2 0
1204.2	1.18E-20	114	118	120	122	123	123	123	123	123	122	122	121	121	7.4206E+01	4.9607E+01	-1.2424E+01	-1 0 -1 0
1204.4	1.15E-20	113	117	120	122	123	124	125	125	125	125	125	125	124	9.2585E+01	3.6544E+01	-1.0167E+01	-1 0 -1 0
1204.6	1.10E-20	115	120	123	125	127	128	128	129	129	129	129	129	129	9.8029E+01	3.7004E+01	-1.0781E+01	-1 0 -1 0
1204.8	1.09E-20	115	119	122	125	126	128	128	129	129	130	130	130	130	1.0296E+02	3.3157E+01	-1.0074E+01	0 -1 0 -1
1205.0	1.08E-20	115	119	122	125	126	128	129	129	130	130	130	130	130	1.0624E+02	3.0748E+01	-9.6483E+00	-1 0 -1 0
1205.2	1.08E-20	115	119	122	124	126	127	128	128	129	129	129	129	129	1.0308E+02	3.2219E+01	-9.8065E+00	-1 0 -2 0
1205.4	1.09E-20	115	120	123	125	126	127	128	128	128	128	128	128	127	9.0920E+01	4.1973E+01	-1.1628E+01	-1 2 -3 1
1205.6	1.10E-20	116	120	123	126	127	128	128	129	129	128	128	128	127	8.5535E+01	4.6894E+01	-1.2613E+01	-2 3 -5 2
1205.8	1.12E-20	115	119	122	124	126	126	127	127	127	127	127	127	126	8.9624E+01	4.1971E+01	-1.1514E+01	-1 3 -4 1
1206.0	1.13E-20	115	119	122	124	126	126	127	127	127	127	127	127	126	8.8153E+01	4.3069E+01	-1.1710E+01	-1 3 -4 1
1206.2	1.13E-20	116	120	123	125	126	127	127	127	127	127	126	126	125	8.0204E+01	4.9655E+01	-1.2964E+01	-1 3 -4 1
1206.4	1.13E-20	116	120	123	125	126	127	127	127	127	127	126	126	125	7.4675E+01	5.4327E+01	-1.3862E+01	-1 2 -3 1
1206.6	1.11E-20	117	122	125	127	128	128	129	128	128	127	127	126	125	6.7350E+01	6.1531E+01	-1.5352E+01	-1 0 -2 0
1206.8	1.09E-20	118	122	125	127	128	129	129	128	128	127	126	125	124	6.0122E+01	6.7439E+01	-1.6468E+01	0 -1 1 -1
1207.0	1.06E-20	119	124	127	129	130	130	130	130	129	128	127	126	125	5.0031E+01	7.7381E+01	-1.8527E+01	0 -2 2 -2
1207.2	1.02E-20	120	125	129	131	132	132	132	132	131	130	129	128	127	5.0364E+01	7.9519E+01	-1.9189E+01	0 -2 1 -1
1207.4	1.00E-20	121	126	129	131	132	133	133	132	131	131	130	129	127	5.2233E+01	7.8515E+01	-1.9055E+01	0 -2 1 -1
1207.6	9.82E-21	120	125	128	131	132	133	133	133	132	132	131	130	130	6.6678E+01	6.7492E+01	-1.7058E+01	0 -1 0 -1
1207.8	9.66E-21	119	124	127	130	131	132	133	133	133	133	133	132	132	8.3345E+01	5.4219E+01	-1.4589E+01	0 -1 1 -1
1208.0	9.53E-21	119	124	128	130	132	133	134	135	135	135	135	134	134	9.0443E+01	5.0080E+01	-1.3986E+01	0 -1 0 -1
1208.2	9.43E-21	119	124	128	131	133	134	135	136	136	136	136	136	136	9.6501E+01	4.6295E+01	-1.3397E+01	0 -1 0 -1
1208.4	9.33E-21	120	125	129	132	134	135	136	137	137	137	137	137	136	9.3305E+01	5.0169E+01	-1.4263E+01	0 -1 0 -1
1208.6	9.27E-21	120	125	129	132	134	136	137	138	138	138	138	138	138	1.0025E+02	4.5634E+01	-1.3529E+01	0 -1 0 -1
1208.8	9.21E-21	120	125	129	133	135	137	138	139	139	139	140	140	140	1.0728E+02	4.1037E+01	-1.2785E+01	-1 0 -1 0
1209.0	9.18E-21	119	125	129	133	135	137	138	139	140	140	141	141	141	1.1369E+02	3.6364E+01	-1.1964E+01	-1 0 -1 0
1209.2	9.18E-21	119	124	129	132	135	136	138	139	140	141	141	141	142	1.2168E+02	2.9875E+01	-1.0742E+01	-1 0 -1 0
1209.4	9.18E-21	119	124	128	132	134	136	138	139	140	141	141	142	142	1.2492E+02	2.7164E+01	-1.0224E+01	-1 0 -1 0
1209.6	9.21E-21	118	124	128	131	134	135	137	139	140	140	141	141	142	1.2811E+02	2.3891E+01	-9.5345E+00	-1 0 -1 0
1209.8	9.23E-21	118	123	127	130	133	135	137	138	139	140	140	141	141	1.2899E+02	2.2313E+01	-9.1445E+00	-1 0 -2 0
1210.0	9.24E-21	117	123	127	130	132	134	136	137	138	139	140	140	141	1.2938E+02	2.1421E+01	-8.9146E+00	-1 0 -2 0
1210.2	9.21E-21	117	122	127	130	132	134	135	137	138	139	140	141	141	1.3158E+02	1.9674E+01	-8.5907E+00	-1 0 -2 0
1210.4	9.18E-21	117	122	126	129	132	134	136	138	139	140	141	141	142	1.3994E+02	1.3008E+01	-7.3498E+00	-1 0 -2 0
1210.6	9.12E-21	116	122	126	129	132	134	136	138	139	141	142	143	143	1.4716E+02	7.6262E+00	-6.3897E+00	-1 1 -2 0
1210.8	9.06E-21	116	121	126	129	132	135	137	138	140	141	142	143	144	1.5343E+02	2.9938E+00	-5.5673E+00	-1 1 -2 0
1211.0	8.96E-21	116	121	126	129	132	135	137	139	141	142	143	145	146	1.5954E+02	-1.3991E+00	-4.8025E+00	-1 1 -2 0
1211.2	8.81E-21	116	122	126	130	133	136	138	140	142	144	145	146	147	1.6461E+02	-3.8406E+00	-4.5242E+00	-1 1 -2 0
1211.4	8.67E-21	117	122	127	131	134	137	140	142	144	145	147	148	149	1.6735E+02	-4.3832E+00	-4.6039E+00	-1 1 -2 0
1211.6	8.46E-21	118	124	129	133	137	140	142	144	146	148	149	151	152	1.6808E+02	-2.0615E+00	-5.3549E+00	-1 1 -2 0
1211.8	8.26E-21	119	126	131	135	139	142	144	147	149	150	152	153	154	1.6706E+02	1.7150E+00	-6.3831E+00	-1 1 -2 0
1212.0	8.07E-21	120	127	132	137	140	144	146	149	151	152	154	155	157	1.7221E+02	-1.3038E-01	-6.2881E+00	-1 1 -2 0
1212.2	7.93E-21	120	127	133	137	141	145	148	150	152	154	156	158	159	1.8017E+02	-4.8645E+00	-5.5841E+00	-1 1 -2 0
1212.4	7.79E-21	120	127	133	138	142	146	149	151	154	156	157	159	160	1.8419E+02	-6.8937E+00	-5.3360E+00	-1 1 -2 0
1212.6	7.68E-21	120	127	133	138	142	146	149	151	154	156	158	159	161	1.8712E+02	-9.1147E+00	-4.9352E+00	-1 1 -2 0
1212.8	7.58E-21	120	127	133	138	142	146	149	152	155	157	159	161	163	1.9811E+02	-1.7453E+01	-3.4299E+00	-1 0 -2 0
1213.0	7.47E-21	120	127	133	138	142	145	149	152	155	157	159	161	163	1.9859E+02	-1.7445E+01	-3.4749E+00	-1 0 -2 0
1213.2	7.39E-21	120	127	133	138	142	145	149	152	155	158	160	162	164	2.0329E+02	-2.1095E+01	-2.8055E+00	-1 0 -1 0
1213.4	7.31E-21	120	127	133	138	142	146	149	152	155	157	160	161	163	1.9924E+02	-1.7832E+01	-3.4166E+00	-1 0 -1 0
1213.6	7.23E-21	120	127	133	138	143	146	150	153	155	157	160	161	163	1.9537E+02	-1.4365E+01	-4.1034E+00	-1 0 -1 0
1213.8	7.16E-21	121	128	134	139	143	147	150	153	156	158	160	162	164	1.9574E+02	-1.4178E+01	-4.1912E+00	0 -1 0 -1
1214.0	7.07E-21	121	128	134	140	144	148	151	155	157	160	162	164	166	2.0042E+02	-1.6219E+01	-3.9972E+00	0 -1 0 -1
1214.2	6.93E-21	122	130	136	142	146	150	154	157	160	162	165	167	168	2.0393E+02	-1.5983E+01	-4.3750E+00	0 -2 1 -1
1214.4	6.80E-21	123	131	138	144	148	153	156	160	163	165	168	170	172	2.0897E+02	-1.6895E+01	-4.5466E+00	0 -2 1 -1
1214.6	6.76E-21	122	130	137	143	148	153	157	161	164	167	169	172	174	2.2237E+02	-2.6960E+01	-2.7411E+00	0 -3 2 -2
1214.8	6.74E-21	122	130	136	142	148	152	156	160	164	167	169	172	174	2.2985E+02	-3.3620E+01	-1.4258E+00	0 -3 3 -2
1215.0	6.71E-21	122	130	136	143	148	153	157	161	164	167	170	173	175	2.3250E+02	-3.5315E+01	-1.1556E+00	1 -4 4 -2
1215.2	6.57E-21	123	132	139	145	150	155	159	163	166	169	172	174	177	2.2525E+02	-2.6492E+01	-3.1325E+00	1 -4 4 -2
1215.4	6.41E-21	126	135	142	148	153	157	161	164	166	169	171	173	175	1.9859E+02	-3.7191E+00	-7.5371E+00	1 -4 4 -2
1215.6	6.23E-21	128	138	145	151	156	160	163	166	168	170	172	173	175	1.7918E+02	1.4618E+01	-1.1264E+01	0 -3 3 -2
1215.8	6.05E-21	131	140	148	154	159	163	165	169	171	173	174	176	177	1.7016E+02	2.5658E+01	-1.3742E+01	0 -3 3 -2
1216.0	5.87E-21	132	142	150	156	161	165	169	172	174	176	178	179	180	1.7425E+02	2.5881E+01	-1.4167E+01	0 -2 2 -1
1216.2	5.75E-21	132	142	150	157	162	167	171	174	177	179	181	183	184	1.9135E+02	1.4646E+01	-1.2339E+01	0 -2 1 -1
1216.4	5.62E-21	132	142	150	157	163	168	172	176	179	182	184	186	188	2.1070E+02	1.3138E+00	-1.0088E+01	0 -1 0 -1
1216.6	5.55E-21	130	140	149	156	162	168	172	177	180	184	187	189	192	2.3726E+02	-1.9812E+01	-8.1617E+00	-1 0 -1 0
1216.8	5.52E-21	127	137	146	154	160	165	172	177	181	185	189	192	195	2.7046E+02	-4.7184E+01	-9.6854E-01	-1 1 -2 0
1217.0	5.48E-21	126	136	145	153	160	166	172	177	182	186	190	194	197	2.8602E+02	-5.9431E+01	1.2937E+00	-1 2 -3 0
1217.2	5.42E-21	126	136	145	153	160	167	173	179	184	189	193	197	201	3.0468E+02	-7.2582E+01	3.5513E+00	-1 2 -3 1
1217.4	5.36E-21	127	137	146	154	162	169	175	181	186	191	195	199	203	3.0799E+02	-7.3026E+01	3.3921E+00	-1 2 -3 1
1217.6	5.31E-21	128	139	148	156	164	171	177	182	187	192	196	200	204	2.9935E+02	-6.4047E+01	1.4921E+00	-1 2 -3 0
1217.8	5.27E-21	130	140	150	158	166	172	178	184	189	193	197	201	204	2.9051E+02	-5.4909E+01	-4.3867E-01	-1 1 -2 0
1218.0	5.22E-21	131	143	152	161	168	174	180	185	190	194	197	201	204	2.7346E+02	-3.9538E+01	-3.4944E+00	-1 0 -1 0
1218.2	5.17E-21	133	145	154	163	170	176	181	186	190	193	197	200	202	2.5300E+02	-2.2007E+01	-6.8906E+00	0 -1 0 -1
1218.4	5.11E-21	135	147	156	164	171	177	182	187	190	194	197	199	202	2.3852E+02	-8.9883E+00	-9.4762E+00	0 -1 0 -1
1218.6	5.01E-21	136	148	158	166	173	179	184	188	192	195	198	201	203	2.3266E+02	-2.2602E+00	-1.0955E+01	0 -1 0 -1
1218.8	4.94E-21	134	146	156	164	171	178	183	188	192	196	200	203	205	2.5934E+02	-2.4322E+01	-6.7614E+00	0 -1 0 -1
1219.0	4.88E-21	131	142	152	161	168	175	181	186	191	196	200	203	207	2.8870E+02	-5.0406E+01	-1.6131E+00	0 -1 0 -1
1219.2	4.80E-21	129	140	150	159	166	174	180	186	191	196	201	205	209	3.1412E+02	-7.1694E+01	2.4611E+00	0 -1 0 -1
1219.4	4.71E-21	126	137	147	156	165	172	179	186	192	198	203	208	213	3.4753E+02	-9.9147E+01	7.6602E+00	0 -1 0 -1
1219.6	4.62E-21	124	134	144	154	162	171	178	185	192	198	204	209	215	3.7313E+02	-1.2101E+02	1.1888E+01	0 -1 0 -1
1219.8	4.52E-21	123	134	144	153	162	170	178	185	192	199	205	210	215	3.8026E+02	-1.2869E+02	1.2947E+01	-1 0 -1 0

TABLE 4-I (CONT.)

ν (cm^{-1})	$\frac{-k_B T}{u}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100 k_B T}{u}$ (θ) / $\frac{k_B T}{u}$ (296) — θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR
1220.0	4.40E-21	125	136	146	155	164	172	180	187	193	199	205	211	216	3.6712E+02	-1.1421E+02	1.0403E+01	-1 1 -3 0
1220.2	4.29E-21	127	139	149	159	168	176	183	190	197	203	209	214	219	3.6478E+02	-1.0794E+02	8.7514E+00	-1 2 -3 1
1220.4	4.16E-21	131	143	154	164	174	182	190	197	204	210	215	221	225	3.6416E+02	-9.9579E+01	6.3304E+00	-1 2 -3 1
1220.6	4.03E-21	134	148	160	170	180	189	196	204	210	216	222	227	232	3.6343E+02	-9.0997E+01	3.8544E+00	-1 2 -3 1
1220.8	3.96E-21	136	150	162	173	183	192	200	208	215	221	227	232	237	3.6995E+02	-9.1103E+01	3.3149E+00	-1 2 -3 1
1221.0	3.93E-21	137	152	164	176	186	195	203	211	218	224	230	236	241	3.7422E+02	-9.1010E+01	2.9133E+00	-1 2 -3 1
1221.2	3.93E-21	138	152	165	176	186	196	204	212	219	225	231	237	242	3.7948E+02	-9.4138E+01	3.3795E+00	-1 2 -3 0
1221.4	4.02E-21	135	149	162	173	183	192	201	209	216	222	229	234	239	3.8493E+02	-1.0249E+02	5.3732E+00	-1 1 -2 0
1221.6	4.15E-21	132	145	157	168	178	187	195	203	210	217	223	229	234	3.8816E+02	-1.1035E+02	7.5912E+00	-1 1 -2 0
1221.8	4.17E-21	132	145	156	167	177	186	194	201	208	215	221	226	232	3.7989E+02	-1.0713E+02	7.1887E+00	-1 1 -2 0
1222.0	4.17E-21	132	145	156	167	177	185	193	201	208	214	220	225	230	3.7382E+02	-1.0301E+02	6.5009E+00	-1 1 -2 0
1222.2	4.11E-21	131	144	156	167	176	186	194	202	209	216	222	228	233	3.9140E+02	-1.1624E+02	8.8772E+00	-1 1 -2 0
1222.4	4.03E-21	130	143	155	166	176	186	195	203	210	218	224	231	236	4.1248E+02	-1.3221E+02	1.1757E+01	-1 0 -1 0
1222.6	3.96E-21	129	142	154	165	176	186	195	204	212	219	227	233	240	4.3490E+02	-1.4967E+02	1.4960E+01	-1 0 -1 0
1222.8	3.84E-21	130	144	156	168	179	189	198	207	216	223	231	237	244	4.4045E+02	-1.4984E+02	1.4525E+01	0 -1 0 -1
1223.0	3.70E-21	132	146	159	171	182	193	203	212	220	228	236	243	249	4.4931E+02	-1.5159E+02	1.4264E+01	0 -1 0 -1
1223.2	3.60E-21	132	146	160	172	184	195	205	215	224	232	240	247	254	4.6801E+02	-1.6358E+02	1.6177E+01	-1 0 -1 0
1223.4	3.53E-21	132	146	160	172	184	195	205	216	225	234	242	249	257	4.8005E+02	-1.7204E+02	1.7625E+01	-1 0 -1 0
1223.6	3.44E-21	132	147	161	174	186	197	208	218	227	236	244	252	260	4.8771E+02	-1.7571E+02	1.8040E+01	-1 0 -1 0
1223.8	3.36E-21	133	148	162	176	188	200	211	222	231	241	249	257	265	5.0277E+02	-1.8371E+02	1.9091E+01	-1 1 -2 0
1224.0	3.30E-21	133	148	163	176	189	201	212	223	232	242	250	259	266	5.0888E+02	-1.8758E+02	1.9698E+01	-1 0 -1 0
1224.2	3.27E-21	133	148	162	176	189	200	212	222	232	241	250	258	266	5.0791E+02	-1.8723E+02	1.9681E+01	-1 0 -1 0
1224.4	3.18E-21	135	152	166	180	193	205	217	227	237	246	255	263	270	5.0389E+02	-1.7806E+02	1.7320E+01	0 -1 0 -1
1224.6	3.12E-21	138	154	169	184	197	209	220	231	240	250	258	266	274	5.0076E+02	-1.7129E+02	1.5589E+01	0 -1 0 -1
1224.8	3.08E-21	139	156	171	186	199	211	223	233	243	252	261	269	276	5.0082E+02	-1.6831E+02	1.4700E+01	-1 0 -1 0
1225.0	3.06E-21	140	156	172	186	199	212	223	234	244	253	262	270	278	5.0482E+02	-1.7051E+02	1.5004E+01	0 -1 0 -1
1225.2	3.02E-21	140	157	173	187	201	213	225	236	246	255	264	272	280	5.0936E+02	-1.7209E+02	1.5072E+01	0 -1 0 -1
1225.4	3.02E-21	14	156	172	187	200	213	224	235	245	255	264	272	280	5.1344E+02	-1.7621E+02	1.5935E+01	-1 0 -1 0
1225.6	3.03E-21	139	155	171	185	199	211	223	234	244	253	262	271	278	5.1597E+02	-1.8002E+02	1.6839E+01	-1 0 -1 0
1225.8	3.03E-21	138	154	170	184	198	210	222	233	243	252	261	270	278	5.1838E+02	-1.8310E+02	1.7550E+01	-1 0 -1 0
1226.0	3.03E-21	137	154	169	183	197	209	221	232	242	252	261	269	277	5.1975E+02	-1.8520E+02	1.8042E+01	-1 0 -1 0
1226.2	2.99E-21	138	154	170	184	198	211	223	234	244	254	263	271	279	5.2699E+02	-1.8913E+02	1.8571E+01	-1 1 -2 0
1226.4	2.93E-21	139	156	172	187	201	214	226	237	248	257	267	275	283	5.3279E+02	-1.8982E+02	1.8267E+01	-1 1 -2 0
1226.6	2.86E-21	142	157	174	189	203	216	229	240	251	261	271	280	288	5.4296E+02	-1.9422E+02	1.8679E+01	-1 0 -1 0
1226.8	2.78E-21	139	157	174	189	204	219	231	244	255	266	276	285	294	5.7400E+02	-2.1583E+02	2.2355E+01	-1 0 -1 0
1227.0	2.71E-21	139	157	174	190	205	220	233	246	258	269	280	290	299	5.9523E+02	-2.3017E+02	2.4725E+01	0 -1 0 -1
1227.2	2.64E-21	142	158	176	193	208	223	237	250	262	273	284	294	304	6.0626E+02	-2.3476E+02	2.5133E+01	0 -1 0 -1
1227.4	2.58E-21	139	157	175	192	208	223	237	250	263	275	286	297	307	6.2644E+02	-2.5062E+02	2.8058E+01	0 -2 1 -1
1227.6	2.52E-21	141	158	176	194	210	225	240	254	267	279	291	302	312	6.4335E+02	-2.6010E+02	2.9382E+01	0 -1 0 -1
1227.8	2.46E-21	139	158	176	194	210	225	241	256	269	282	294	305	316	6.6291E+02	-2.7420E+02	3.1842E+01	0 -1 0 -1
1228.0	2.41E-21	139	158	176	194	211	227	242	257	271	283	296	307	318	6.7292E+02	-2.8100E+02	3.2978E+01	0 -2 1 -1
1228.2	2.35E-21	139	158	177	196	213	230	246	261	275	289	301	314	325	6.9859E+02	-2.9715E+02	3.5512E+01	0 -1 0 -1
1228.4	2.30E-21	141	161	180	199	217	234	250	265	280	293	306	318	330	7.0125E+02	-2.9425E+02	3.4419E+01	0 -1 0 -1
1228.6	2.27E-21	142	162	182	201	219	236	252	267	281	295	308	320	331	6.9918E+02	-2.9017E+02	3.3392E+01	-1 0 -1 0
1228.8	2.25E-21	144	165	185	204	222	239	255	270	284	297	310	322	333	6.9113E+02	-2.8028E+02	3.1170E+01	-1 0 -1 0
1229.0	2.24E-21	146	167	187	206	224	241	257	272	286	299	311	323	334	6.8017E+02	-2.6922E+02	2.8857E+01	-1 1 -2 0
1229.2	2.25E-21	146	167	187	206	224	240	256	271	285	298	310	321	332	6.7190E+02	-2.6334E+02	2.7842E+01	-1 2 -3 0
1229.4	2.27E-21	144	165	184	203	220	237	253	267	281	294	306	318	329	6.7285E+02	-2.6836E+02	2.9242E+01	-1 1 -2 0
1229.6	2.28E-21	142	162	181	200	217	234	249	264	278	291	303	315	326	6.7688E+02	-2.7540E+02	3.0975E+01	-1 0 -1 0
1229.8	2.28E-21	141	161	180	198	215	232	248	262	276	289	302	314	325	6.8117E+02	-2.8108E+02	3.2281E+01	0 -1 0 -1
1230.0	2.27E-21	141	160	180	198	215	232	248	263	277	290	303	314	326	6.8733E+02	-2.8567E+02	3.3098E+01	0 -2 1 -1
1230.2	2.21E-21	142	162	181	200	219	235	252	268	282	296	309	322	333	7.1101E+02	-2.9915E+02	3.5014E+01	0 -2 1 -1
1230.4	2.14E-21	142	163	183	203	222	240	257	273	289	303	317	330	342	7.4378E+02	-3.1917E+02	3.8054E+01	0 -2 1 -1
1230.6	2.08E-21	143	165	186	206	226	245	261	280	296	311	326	339	352	7.7435E+02	-3.3655E+02	4.0537E+01	0 -2 1 -1
1230.8	2.02E-21	143	165	187	208	228	248	266	284	301	317	332	346	359	8.0194E+02	-3.5417E+02	4.3335E+01	0 -2 1 -1
1231.0	1.97E-21	144	166	188	210	230	250	269	287	303	319	334	349	362	8.0684E+02	-3.5518E+02	4.3202E+01	0 -2 1 -1
1231.2	1.92E-21	144	166	189	211	232	252	271	289	307	323	339	354	368	8.3100E+02	-3.7155E+02	4.5933E+01	0 -2 1 -1
1231.4	1.86E-21	144	167	191	212	233	254	273	292	310	326	342	357	372	8.4370E+02	-3.7882E+02	4.6970E+01	0 -2 1 -1
1231.6	1.81E-21	145	168	192	214	236	257	277	296	314	331	347	362	377	8.5602E+02	-3.8450E+02	4.7571E+01	0 -2 1 -1
1231.8	1.75E-21	146	172	196	219	241	262	282	301	319	336	352	367	382	8.5334E+02	-3.7983E+02	4.5240E+01	0 -1 0 -1
1232.0	1.71E-21	149	174	198	222	245	266	287	307	325	343	360	375	390	8.8086E+02	-3.9162E+02	4.7504E+01	-1 0 -1 0
1232.2	1.67E-21	149	174	198	223	246	269	290	311	330	348	366	382	398	9.1394E+02	-4.1425E+02	5.1303E+01	-1 1 -2 0
1232.4	1.65E-21	151	177	202	227	251	273	295	315	334	353	370	386	402	9.1164E+02	-4.0683E+02	4.9310E+01	-1 2 -2 0
1232.6	1.64E-21	154	180	205	229	253	275	296	316	335	353	369	385	400	8.8696E+02	-3.8554E+02	4.5169E+01	-1 2 -2 0
1232.8	1.64E-21	155	181	206	230	253	275	296	315	334	351	368	383	398	8.6664E+02	-3.6944E+02	4.2184E+01	-1 1 -2 0
1233.0	1.64E-21	155	181	206	230	253	275	296	315	333	351	367	382	397	8.6187E+02	-3.6607E+02	4.1605E+01	-1 0 -1 0
1233.2	1.65E-21	155	181	206	231	253	275	296	315	333	350	367	382	396	8.5946E+02	-3.6411E+02	4.1236E+01	0 -1 0 -1
1233.4	1.65E-21	154	180	205	229	252	274	294	314	332	350	366	382	396	8.7078E+02	-3.7473E+02	4.3386E+01	0 -2 0 -1
1233.6	1.64E-21	151	177	202	226	250	272	293	313	332	350	367	383	399	8.9813E+02	-3.9794E+02	4.7861E+01	0 -2 1 -1
1233.8	1.62E-21	151	176	202	227	251	274	295	316	336	354	372	389	404	9.2488E+02	-4.1647E+02	5.1001E+01	0 -2 1 -1
1234.0	1.57E-21	154	180	207	232	256	280	302	323	343	361	379	396	412	9.3091E+02	-4.1345E+02	4.9581E+01	0 -2 1 -1
1234.2	1.52E-21	158	183	210	236	261	284	307	328	348	367	385	402	418	9.4367E+02	-4.1750E+02	4.9661E+01	0 -2 1 -1
1234.4	1.47E-21	159	185	213	239	264	288	311	332	353	372	390	407	423	9.4913E+02	-4.1680E+02	4.8975E+01	0 -2 1 -1
1234.6	1.44E-21	159	187	214	241	266	290	313	335	355	374	392	410	426	9.5154E+02	-4.1613E+02	4.8565E+01	0 -1 0 -1
1234.8	1.40E-21	159	187	215	242	268	292	315	338	359	378	397	414	431	9.7071E+02	-4.2816E+02	5.0448E+01	0 -2 1 -1
1235.0	1.35E-21	161	190	219	247	274	299	323	345	367	387	406	424	441	9.9245E+02	-4.3697E+02	5.1149E+01	0 -1 0 -1
1235.2	1.32E-21	162	192	221	250	277	303	328	351	373	393	413	432	449	1.0190E+03	-4.5217E+02	5.3304E+01	0 -1 0 -1
1235.4	1.28E-21	164	195	225	254	282	308	333	357	379	400	420	439	457	1.0345E+03	-4.5780E+02	5.3632E+01	0 -1 0 -1
1235.6	1.25E-21	165	196	227	256	285	312	338	362	385	407	427	447	465	1.0624E+03	-4.7416E+02	5.6030E+01	-1 0 -1 0
1235.8	1.23E-21	164	196	227	256	285	313	339	363	387	409	429	449	468	1.0765E+03	-4.8423E+02	5.7777E+01	-1 0 -1 0
1236.0	1.21E-21	165	196	227	257	286	313	339	363	386	408	428	448	466	1.0634E+03	-4.7392E+02	5.5871E+01	-1 0 -1 0
1236.2	1.20E-21	165	198	229	259	287	314	340	364	387	408	429	448	466	1.0537E+03	-4.6485E+02	5.4036E+01	-1 0 -1 0
1236.4	1.20E-21	166	197	228	258	287	314	339	364	386	408	428	448	466	1.0576E+03	-4.6839E+02	5.4747E+01	-1 0 -1 0
1236.6	1.20E-21	165	197	228	257	286	313	339	363	386	408	429	448	467	1.0651E+03	-4.7468E+02	5.5951E+01	-1 0 -1 0
1236.8	1.20E-21	164	195	226	257	285	313	339	364	387	409	430	450	469	1.0821E+03	-4.8826E+02	5.8478E+01	-1 0 -1 0

TABLE 4-I (CONT.)

ν (cm^{-1})	$\frac{-L_T}{u}$ ($\frac{cm^2}{molecule}$) θ=296K	$\frac{100 L_T}{u}$ (θ) / $\frac{L_T}{u}$ (296) — θ (Temperature in Kelvins) 350	375	400	425	450	475	500	525	550	575	600	625	650	COEFFICIENT a_0	a_1	a_2	% ERROR	
1237.0	1.20E-21	164	194	225	255	284	312	339	364	388	411	432	453	472	1.1873E+03	-5.0821E+02	8.2174E+01	0 -1	0 -1
1237.2	1.19E-21	161	191	222	253	283	311	339	364	388	412	434	455	474	1.1331E+03	-5.2978E+02	8.6384E+01	0 -2	1 -1
1237.4	1.18E-21	158	189	220	250	280	309	336	362	386	410	432	453	473	1.1425E+03	-5.4022E+02	8.8568E+01	1 -3	1 -1
1237.6	1.16E-21	157	188	219	250	279	309	336	362	387	411	433	455	475	1.1566E+03	-5.5158E+02	7.0695E+01	1 -3	2 -1
1237.8	1.13E-21	154	186	218	249	279	309	336	363	388	413	436	458	478	1.1819E+03	-5.7118E+02	7.4280E+01	1 -3	2 -1
1238.0	1.10E-21	156	188	220	252	283	313	342	369	396	421	445	468	489	1.2206E+03	-5.9505E+02	7.7956E+01	1 -3	2 -1
1238.2	1.08E-21	157	189	222	255	287	319	349	377	405	431	456	480	502	1.2678E+03	-6.2413E+02	8.2444E+01	1 -3	2 -1
1238.4	1.02E-21	157	190	224	258	291	324	355	385	413	440	466	491	514	1.3123E+03	-6.5215E+02	8.6816E+01	1 -3	1 -1
1238.6	9.95E-22	158	191	226	260	294	328	359	390	419	447	474	499	523	1.3452E+03	-6.7263E+02	9.0001E+01	0 -2	1 -1
1238.8	9.72E-22	158	192	227	262	297	330	363	394	424	452	479	504	529	1.3647E+03	-6.8393E+02	9.1639E+01	1 -3	1 -1
1239.0	9.53E-22	158	192	227	263	298	332	365	397	427	456	484	510	535	1.3715E+03	-7.0213E+02	9.4677E+01	1 -3	2 -1
1239.2	9.35E-22	158	192	228	264	300	334	368	400	431	460	488	515	540	1.4145E+03	-7.1741E+02	9.7184E+01	1 -4	2 -1
1239.4	9.14E-22	159	194	231	267	304	339	373	406	437	467	495	522	548	1.4331E+03	-7.2595E+02	9.8085E+01	1 -4	2 -1
1239.6	9.04E-22	159	194	231	268	304	340	374	407	438	468	496	523	549	1.4384E+03	-7.2924E+02	9.8593E+01	1 -3	2 -1
1239.8	8.93E-22	160	195	232	269	306	341	375	408	440	469	498	525	551	1.4389E+03	-7.2748E+02	9.8057E+01	1 -3	2 -1
1240.0	8.80E-22	161	197	234	271	308	344	378	411	443	473	502	529	555	1.4466E+03	-7.3027E+02	9.8172E+01	1 -3	1 -1
1240.2	8.67E-22	162	199	236	274	311	347	382	415	447	478	507	534	560	1.4583E+03	-7.3487E+02	9.8514E+01	1 -2	1 -1
1240.4	8.54E-22	163	200	238	276	314	350	385	419	451	482	511	539	565	1.4703E+03	-7.4042E+02	9.9108E+01	0 -2	1 -1
1240.6	8.37E-22	165	203	241	280	318	354	391	424	456	487	516	544	571	1.4778E+03	-7.4184E+02	9.8627E+01	0 -2	1 -1
1240.8	8.20E-22	166	204	244	283	321	359	395	429	462	493	523	551	578	1.4983E+03	-7.5137E+02	9.9896E+01	0 -1	0 -1
1241.0	8.06E-22	165	203	243	282	321	359	396	431	464	496	526	555	583	1.5261E+03	-7.7236E+02	1.0367E+02	0 -2	1 -1
1241.2	7.79E-22	166	205	246	286	326	365	403	439	474	507	538	568	596	1.5715E+03	-7.9924E+02	1.0769E+02	0 -2	1 -1
1241.4	7.54E-22	168	208	249	291	332	372	411	448	483	517	549	580	609	1.6134E+03	-8.2314E+02	1.1105E+02	1 -3	1 -1
1241.6	7.33E-22	168	209	251	294	336	377	417	455	491	526	559	591	621	1.6569E+03	-8.5027E+02	1.1527E+02	1 -3	2 -1
1241.8	7.18E-22	167	208	251	295	338	381	420	459	496	532	566	598	629	1.6952E+03	-8.7692E+02	1.1980E+02	1 -4	2 -1
1242.0	7.03E-22	166	208	251	295	339	381	423	462	501	537	572	605	636	1.7298E+03	-9.0122E+02	1.2397E+02	2 -4	3 -2
1242.2	6.89E-22	166	207	251	295	339	382	424	464	502	539	574	608	640	1.7478E+03	-9.1348E+02	1.2608E+02	2 -5	3 -2
1242.4	6.75E-22	165	207	253	295	339	383	425	465	504	541	577	611	643	1.7661E+03	-9.2747E+02	1.2855E+02	2 -5	3 -2
1242.6	6.58E-22	166	209	253	299	344	388	431	472	512	550	586	621	654	1.7989E+03	-9.4993E+02	1.3114E+02	2 -5	3 -2
1242.8	6.46E-22	166	209	254	301	347	392	435	478	518	557	594	629	663	1.8358E+03	-9.6994E+02	1.3501E+02	2 -4	2 -1
1243.0	6.33E-22	168	211	257	304	351	397	441	484	524	564	601	637	671	1.8565E+03	-9.7990E+02	1.3615E+02	1 -4	2 -1
1243.2	6.20E-22	171	215	261	309	356	402	447	490	531	570	608	644	678	1.8648E+03	-9.7928E+02	1.3525E+02	1 -3	2 -1
1243.4	6.07E-22	173	218	265	313	361	407	452	495	537	576	614	650	684	1.8708E+03	-9.7713E+02	1.3410E+02	1 -3	1 -1
1243.6	5.94E-22	175	221	269	318	366	412	458	501	543	582	620	656	691	1.8772E+03	-9.7569E+02	1.3309E+02	1 -2	1 -1
1243.8	5.84E-22	177	224	273	322	370	417	463	507	549	589	627	664	698	1.8936E+03	-9.8216E+02	1.3357E+02	0 -2	1 -1
1244.0	5.73E-22	179	226	275	325	374	422	468	512	554	595	633	670	705	1.9082E+03	-9.8820E+02	1.3408E+02	0 -2	1 -1
1244.2	5.66E-22	178	225	274	324	373	421	467	512	554	595	634	670	705	1.9171E+03	-9.9570E+02	1.3554E+02	1 -2	1 -1
1244.4	5.58E-22	178	225	274	324	373	421	468	512	555	595	634	671	706	1.9208E+03	-9.9751E+02	1.3580E+02	1 -3	1 -1
1244.6	5.49E-22	177	224	274	324	373	422	468	513	556	597	637	674	709	1.9390E+03	-1.0119E+03	1.3837E+02	1 -3	1 -1
1244.8	5.39E-22	176	223	273	324	374	423	471	517	560	602	642	681	717	1.9780E+03	-1.0398E+03	1.4325E+02	1 -3	1 -1
1245.0	5.27E-22	175	223	274	325	377	427	476	522	567	610	651	690	728	2.0267E+03	-1.0728E+03	1.4875E+02	1 -3	2 -1
1245.2	5.16E-22	174	222	274	326	379	430	480	528	574	618	660	700	738	2.0766E+03	-1.1074E+03	1.5460E+02	1 -3	2 -1
1245.4	5.02E-22	174	223	276	329	383	435	486	535	582	628	671	712	751	2.1258E+03	-1.1387E+03	1.5956E+02	1 -3	2 -1
1245.6	4.86E-22	175	225	278	333	388	443	495	545	594	640	685	727	768	2.1892E+03	-1.1789E+03	1.6591E+02	1 -4	2 -1
1245.8	4.70E-22	174	225	280	337	393	449	503	555	606	654	700	744	786	2.2671E+03	-1.2305E+03	1.7436E+02	1 -4	2 -1
1246.0	4.58E-22	173	224	280	338	397	454	510	564	616	666	714	760	804	2.3487E+03	-1.2869E+03	1.8390E+02	2 -4	2 -1
1246.2	4.45E-22	172	226	283	342	402	461	519	574	628	679	729	776	821	2.4145E+03	-1.3287E+03	1.9052E+02	2 -4	2 -1
1246.4	4.33E-22	173	227	286	346	407	468	527	584	639	691	742	790	836	2.4711E+03	-1.3640E+03	1.9600E+02	2 -4	2 -1
1246.6	4.25E-22	173	227	286	347	409	472	529	587	643	696	747	796	842	2.4995E+03	-1.3831E+03	1.9918E+02	2 -4	2 -1
1246.8	4.18E-22	175	230	289	351	413	474	534	592	647	701	752	801	848	2.5059E+03	-1.3829E+03	1.9855E+02	2 -4	2 -1
1247.0	4.17E-22	175	229	288	349	411	471	531	588	643	696	747	795	841	2.4898E+03	-1.3669E+03	1.9597E+02	2 -4	2 -1
1247.2	4.18E-22	174	227	285	345	405	465	523	580	634	686	736	784	829	2.4423E+03	-1.3458E+03	1.9289E+02	2 -4	2 -1
1247.4	4.15E-22	173	225	283	342	402	461	519	574	628	679	729	776	821	2.4156E+03	-1.3298E+03	1.9074E+02	2 -4	2 -1
1247.6	4.14E-22	174	227	285	345	406	465	523	579	634	686	735	783	828	2.4372E+03	-1.3412E+03	1.9221E+02	2 -4	2 -1
1247.8	4.09E-22	173	226	285	345	406	467	524	583	637	690	741	789	835	2.4705E+03	-1.3648E+03	1.9827E+02	2 -4	2 -1
1248.0	4.03E-22	171	225	283	344	406	467	526	584	639	693	744	792	839	2.5001E+03	-1.3877E+03	2.0047E+02	2 -5	2 -1
1248.2	3.94E-22	171	225	285	347	409	471	532	591	648	702	754	804	852	2.5512E+03	-1.4210E+03	2.0584E+02	2 -5	3 -1
1248.4	3.84E-22	170	225	286	349	413	476	539	599	657	712	766	817	866	2.6127E+03	-1.4623E+03	2.1268E+02	3 -6	3 -2
1248.6	3.74E-22	170	225	287	352	417	482	545	607	666	724	779	831	881	2.6784E+03	-1.5061E+03	2.1990E+02	3 -6	3 -2
1248.8	3.65E-22	169	225	288	354	421	487	552	616	677	736	792	846	898	2.7518E+03	-1.5558E+03	2.2817E+02	3 -6	4 -2
1249.0	3.54E-22	168	225	290	357	426	494	561	626	689	749	807	863	916	2.8292E+03	-1.6071E+03	2.3657E+02	3 -6	4 -2
1249.2	3.46E-22	167	225	290	359	428	498	566	632	696	758	817	874	928	2.8827E+03	-1.6435E+03	2.4266E+02	3 -6	3 -2
1249.4	3.38E-22	166	224	289	359	429	501	569	637	702	765	825	883	939	2.9383E+03	-1.6836E+03	2.4968E+02	3 -6	3 -2
1249.6	3.31E-22	165	221	287	357	428	501	570	639	705	769	831	890	946	2.9901E+03	-1.7237E+03	2.5701E+02	3 -6	4 -2
1249.8	3.23E-22	161	219	286	356	429	502	573	643	710	775	838	898	955	3.0410E+03	-1.7688E+03	2.6351E+02	3 -7	4 -2
1250.0	3.14E-22	164	223	291	363	436	510	582	653	721	787	850	911	969	3.0723E+03	-1.7744E+03	2.6480E+02	3 -7	4 -2

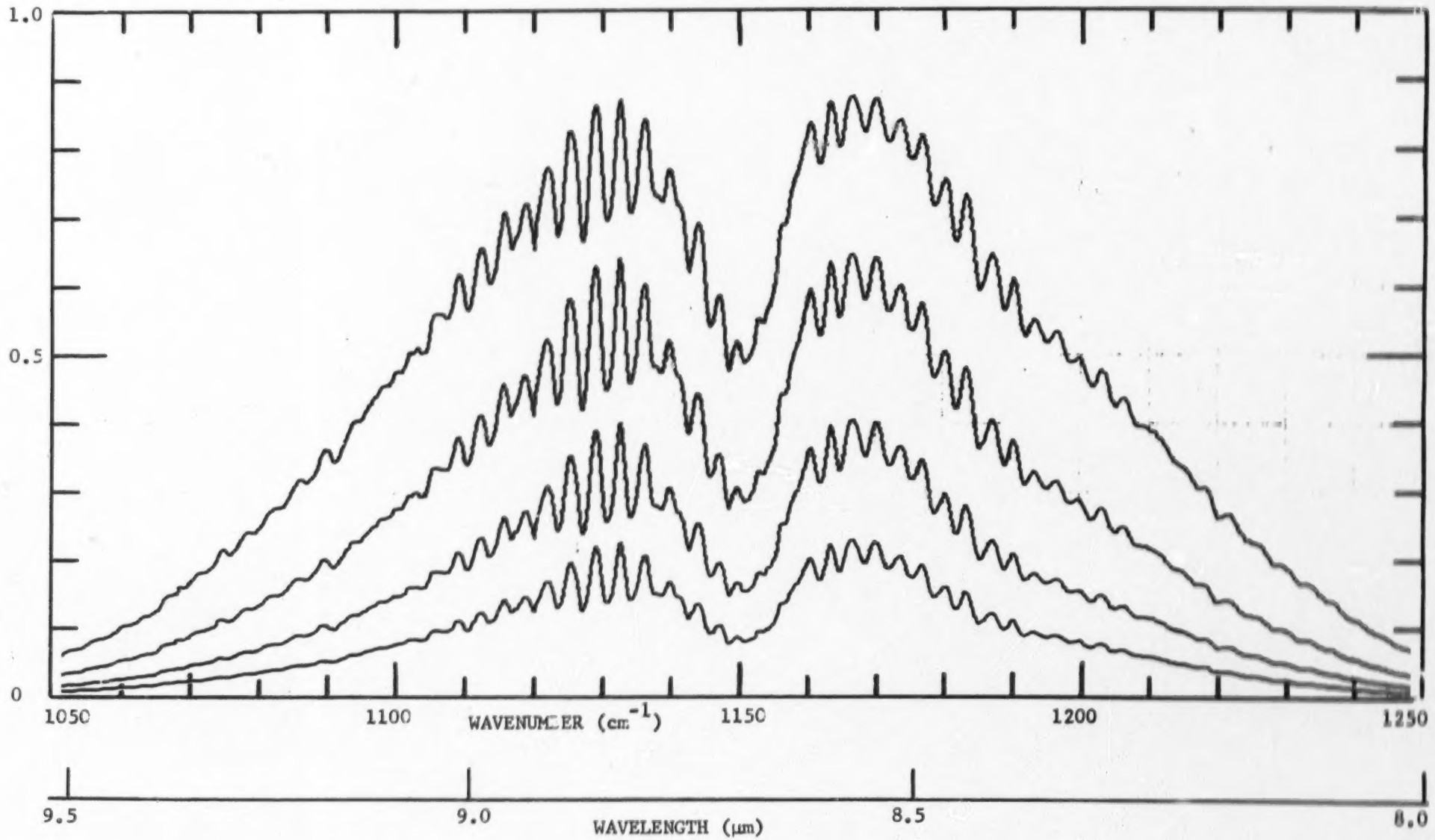

FIG. 4-1. Spectral curves of calculated emissivity for SO_2 at 475 K. The curves correspond to 1 cm^{-1} spectral slitwidth and represent samples with equivalent pressures near 1 atm. Absorber thicknesses in molecules cm^{-2} from top curve to bottom are: 4×10^{19}, 2×10^{19}, 1×10^{19} and 0.5×10^{19}.

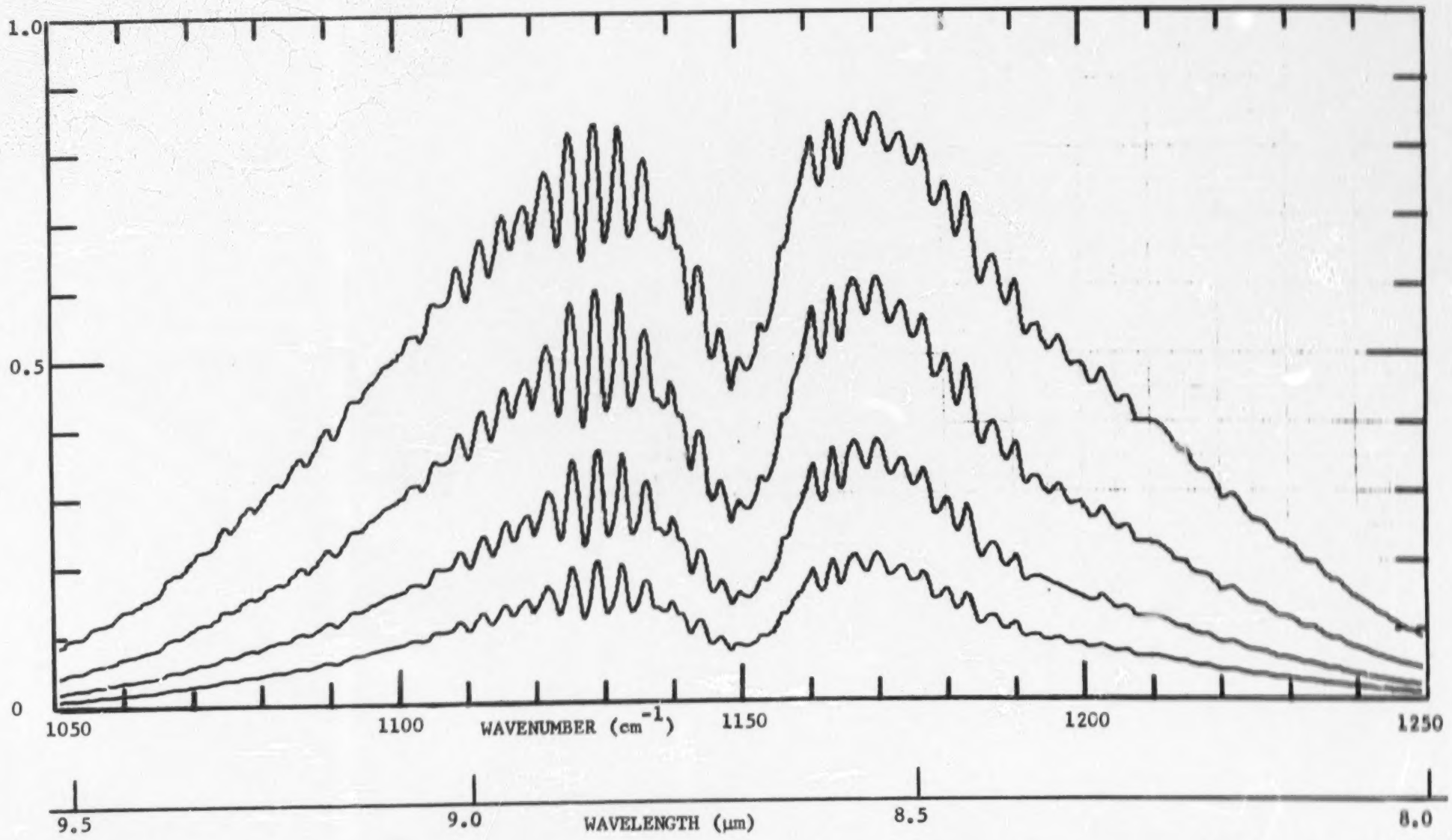

FIG. 4-2. Spectral curves of calculated emissivity for SO_2 at 550 K. The curves correspond to 1 cm^{-1} spectral slitwidth and represent samples with equivalent pressures near 1 atm. Absorber thicknesses in molecules cm^{-2} from top curve to bottom are: 4×10^{19}, 2×10^{19}, 1×10^{19} and 0.5×10^{19}.

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SECTION 5

EXPERIMENTAL RESULTS FOR H_2O

Spectral curves of transmittance for H_2O between 1000 and 1300 cm^{-1} are shown in Fig. 5-1. Many additional lines not apparent in the figure also occur in this region.

The parameters for more than 600 individual lines between 1000 and 1300 cm^{-1} have been tabulated by Calfee and Benedict[2]. The parameters listed for each line include the identification of the upper and lower states involved in the transition, the wavenumber position of the line center, the strength, and the half-width. The values tabulated are based on a combination of theory and experiment. The positions are known to approximately 0.01 cm^{-1} for most of the lines strong enough to be significant for smokestack monitoring. However, the strengths and widths should be checked experimentally and adjustments made to provide fits with experimental data. The temperature dependence of the strengths and widths can be calculated reliably after these quantities have been determined at one temperature.

A relatively smooth envelope curve can be drawn through points of maximum transmittance in the curves of Fig. 5-1. Such a curve would occur between transmittances of 0.70 and 0.80 in the middle panel of Fig. 5-1. Continuum absorption is the cause of this "extra" absorption not due to the nearby

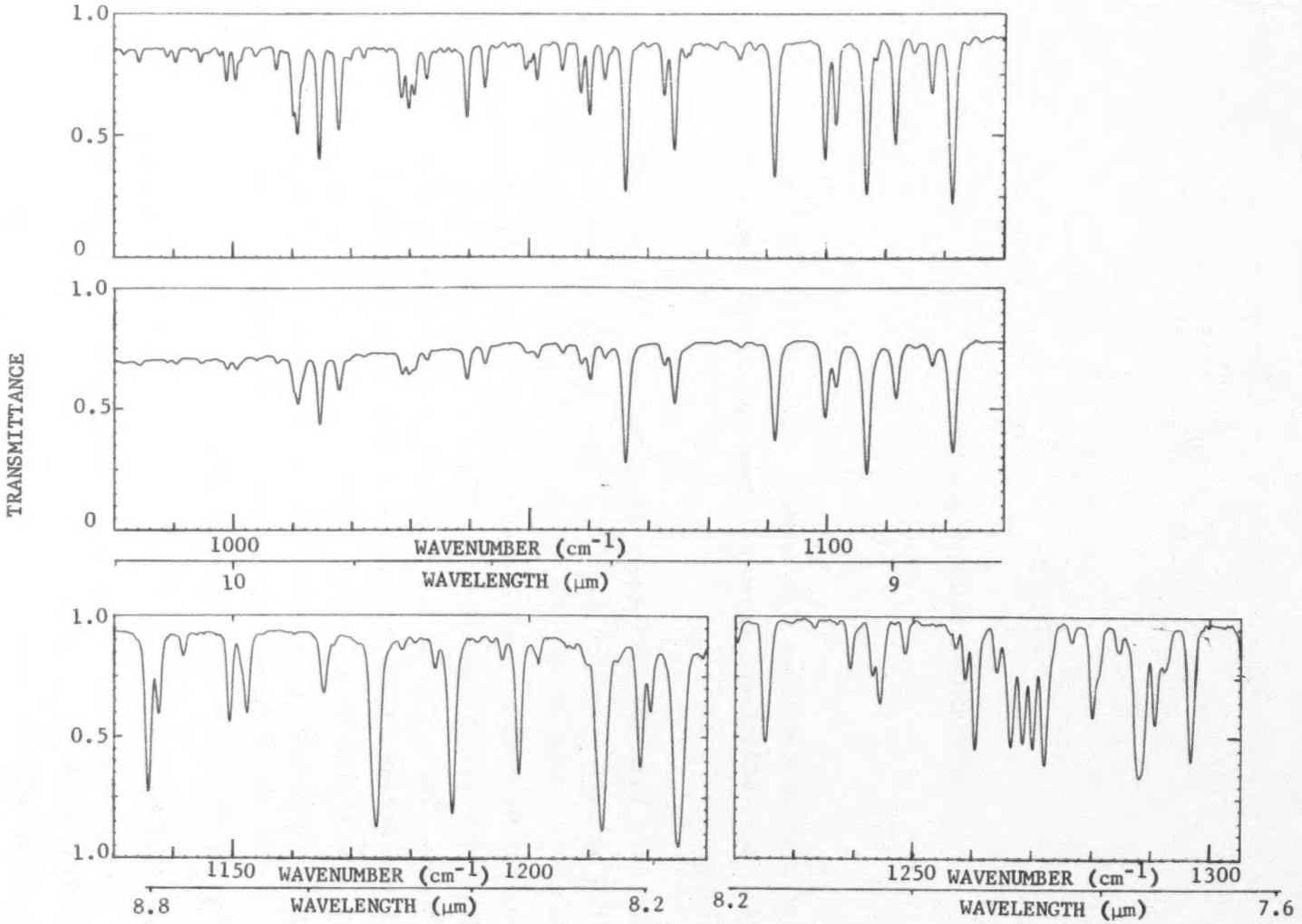

FIG. 5-1. Spectral curves for pure H_2O between 980 and 1300 cm^{-1}. The sample parameters are:

Curve	L (cm)	p (atm)	u (molecules cm^{-2})	Temp. (Kelvins)	Slitwidth (cm^{-1})
Upper	2880	0.252	13.5 E21	392	0.6
Middle	416	1.00	7.78 E21	392	0.6
Lower Left	416	0.504	3.91 E21	392	0.8
Lower Right	416	0.132	1.02 E21	392	1.0

lines. It may be due to the extreme wings of very strong lines centered below 1000 cm^{-1} and above 1300 cm^{-1} or to H_2O dimers. The continuum absorption coefficient at a given wavenumber varies with pressure according to the following equation for an $H_2O + N_2$ mixture.

$$(-1/u)\ln T \text{ (continuum)} = C = C_s^o\, p + C_{N_2}^o\, p_{N_2} . \qquad (5\text{-}1)$$

The transmittance refers to the continuum only; p and p_{N_2} are the pressures, in atm, of the H_2O and N_2, respectively. The subscript s denotes self-broadening; i.e., continuum due to broadening by collisions of the absorbing H_2O molecules with other H_2O molecules. Similarly, the subscript N_2 corresponds to collisions of the H_2O molecules with N_2. In the smokestack exhaust or in the atmospheric path, collisions of H_2O can be treated as if they were with N_2. The quantity $-\ln T$ (continuum) for a pure sample is proportional to pu and, thus, to p^2 for a cell of given length. The strong dependence on p can be seen by comparing the upper and middle panels of Fig. 5-1. The 1 atm sample represented by the middle panel shows more continuum absorption than the 0.252 atm sample represented by the upper panel in spite of the larger absorber thickness of the 0.252 sample.

We have assumed that the continuum is due to the extreme wings of lines, rather than to dimers. For the purposes of analysis, it does not matter which is the true absorbing mechanism since the pressure dependence indicated by Eq. (5-1) is valid for both. Values of C_s^o and $C_{N_2}^o$ calculated on the basis the Lorentz line shape for all of the lines outside the 1000-1300 cm^{-1} interval do not agree with experimental values. This result does not exclude the wings of these lines as the cause of the absorption, but it does indicate that the Lorentz shape is not valid in the extreme wings. Values of $C_{N_2}^o$ are so small that they are difficult to determine experimentally, but they are probably less than 0.005 C_s^o and much less than the calculated values. The exhaust from a typical smokestack contains several percent H_2O so that the self-broadening term in Eq. (5-1) is dominant. We have recently measured C_s^o from samples of pure H_2O at

392 K. The following results were obtained:

Wavenumber (cm^{-1})	C_s^o (molecules^{-1} cm^2 atm^{-1})
1000	40×10^{-24}
1100	30×10^{-24}
1200	43×10^{-24}
1250	70×10^{-24}

The H_2O data obtained as part of the present study combined with those obtained in our laboratory under other contracts are all of the laboratory data on H_2O that are required to account for this gas in the reduction of data on smokestack exhausts. We recommended that these data be used to determine the continuum coefficients and to adjust the line parameters tabulated by Benedict and Calfee. Relatively simple computer programs can then be used to calculate the emission by any exhaust gas and the absorption by any atmospheric path of interest.

SECTION 6

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APPENDIX A

This appendix provides factors required to convert units of temperature, absorber thickness, and strengths of lines or bands used in this report to units commonly used by other workers. The absorber thickness u is the number of molecules of the absorbing gas per cm^2 cross section of the optical path. For a perfect gas, the number N of molecules of absorbing gas per cm^3 is:

$$N = 0.269 \times 10^{20} \; p \; (273 \; K/\theta) \; ,$$

where θ is the temperature in Kelvin and p is the partial pressure of the absorbing gas in atm. It follows that:

$$u \text{ (molecules cm}^{-2}\text{)} = N \text{ (molecules cm}^{-3}\text{)} L \text{ (cm)} = 0.269 \times 10^{20} \; pL \; (273.2 \; K/\theta) \; .$$

Units of $(\text{atm} \cdot \text{cm})_{STP}$ are used frequently by other workers for a quantity corresponding to our absorber thickness:

$$u \; (\text{atm} \cdot \text{cm})_{STP} = (273.2 \; K/\theta) \; p(\text{atm}) \; L(\text{cm}) \; .$$

The subscript STP indicates that the absorber pressure p has been adjusted to the value it would be if N were kept constant and θ were standard temperature, 273.2 K.

The unit

$$u(\text{atm} \cdot \text{cm})_{300\ \text{K}} = (300\ \text{K}/\theta)\ p(\text{atm})\ L(\text{cm})$$

also appears in the scientific literature. At θ = 300 K, a common laboratory temperature, this unit conveniently becomes p(atm) L(cm). The units defined in the equations above differ from each other by factors which are independent of temperature. The factors are summarized in Table A-1.

Some workers use units equivalent to

$$u(\text{atm} \cdot \text{cm})_{\text{at temp.}} = p(\text{atm})\ L(\text{cm}) .$$

It is apparent that the conversion factor relating this quantity to our molecules cm^{-2} depends on temperature. The constants required to make the conversion are given in Table A-2 for several temperatures. As explained in Section 1, deviations from the perfect gas law must be accounted for at high pressure.

Units of gms of absorbing gas per cm^2 also are used. Table A-1 relates absorber thicknesses in these units for SO_2 and H_2O to molecules cm^{-2}. The conversion between these sets of units is independent of temperature, but dependent on the molecular weight of the absorber (18 for H_2O and 64 for SO_2). Since the density of liquid water is 1 gm/cm^3, values of u in gm H_2O cm^{-2} are numerically equivalent to those in precipitable cm (pr.cm) which correspond to the depth of the column of liquid water that would result if the H_2O vapor in the optical path were condensed.

The units of absorption coefficient κ are the reciprocals of the units of absorber thickness. The strength of a line or band is the integral of the absorption coefficient, $\int \kappa\, d\nu$, where the integration is performed over the line or band. It follows that the units of strength are cm^{-1} times the reciprocal of the units of absorber thickness. In Tables A-1 and A-2, the unit cm^{-1} which denotes the number of waves per cm is kept separate from the unit cm which denotes length. Some workers integrate over a line or band in units of sec^{-1} instead of cm^{-1}. In this case,

sec^{-1} is the number of waves per second; thus, values expressed in the two different sets of units differ by c, the speed of light in cm sec^{-1}.

TABLE A-1

CONVERSION FACTORS FOR ABSORBER THICKNESSES AND STRENGTHS VALID AT ALL TEMPERATURES

Absorber Thickness Equivalent of 10^{20} molecules cm^{-2}	Strengths of Lines or Bands Equivalent of 10^{-20} molecules^{-1} cm^2 cm^{-1}
3.72 $(atm\ cm)_{STP}$ (for all gases)	0.269 $(atm\ cm)^{-1}_{STP} \cdot cm^{-1}$
4.09 $(atm\ cm)_{300\ K}$ (for all gases)	0.245 $(atm\ cm)^{-1}_{300\ K} \cdot cm^{-1}$
0.01063 gm SO_2/cm^2	94.1 $(gm\ SO_2)^{-1}\ cm^2 \cdot cm^{-1}$
0.00299 gm H_2O/cm^2 or (pr.cm)	335 $(gm\ H_2O)^{-1}\ cm^2 \cdot cm^{-1}$ or $(pr.cm)^{-1}\ cm^2 \cdot cm^{-1}$

TABLE A-2

CONVERSION OF TEMPERATURE SCALES AND ABSORBER THICKNESS

Temperatures				Equivalent of 10^{20} molecules cm^{-2} $(atm\ cm)_{at\ temp.}$
Kelvin	Centigrade	Fahrenheit	Rankine	
273.2	0	32.0	491.7	3.72
296	22.8	73.1	532.7	4.04
300	26.8	80.2	539.9	4.09
325	51.8	125.2	584.9	4.43
350	76.8	170.2	629.9	4.77
375	101.8	215.2	674.9	5.11
400	126.8	260.2	719.9	5.45
425	151.8	305.2	764.9	5.80
450	176.8	350.2	809.9	6.14
475	201.8	395.2	844.9	6.48
500	226.8	440.2	899.9	6.81
525	251.8	485.2	944.9	7.16
550	276.8	530.2	989.9	7.50
575	301.8	575.2	1034.9	7.84
600	326.8	620.2	1079.9	8.18
625	351.8	665.2	1124.9	8.52
650	376.8	710.2	1169.9	8.86